Research Accomplishments

FOR THE

Environmental Management Science Program

1999 Year-End Summary

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RESEARCH ACCOMPLISHMENTS FOR THE ENVIRONMENTAL MANAGEMENT SCIENCE PROGRAM

Introduction

The intent of this document is to provide information concerning the research transition activities of the Environmental Management Science Program (EMSP). Research transitions are measures of how successfully the program has transitioned knowledge gained from research projects to other areas. These measures may be in the form of actual transfers of new knowledge or data gained through research products or processes to other areas within EM, such as Focus Areas and Crosscutting Programs, or may be more general knowledge transfer measures found in similar research programs, such as collaborations, numbers of student researchers, peer reviewed papers and presentations (communication products), or consultations.

The information contained in this document has been gathered from various sources, such as interactions with EMSP staff, proceedings from EMSP workshops and technical conferences, principal investigators, the Project Tracking System, EMSP Project Annual Reports, and literature searches. The information presented is an attempt to capture research transition activities and therefore should not be considered to be a complete or accurate listing. This volume contains the best available data as of December 31, 1999. Where incomplete information was received, efforts are underway to rectify this situation, as well as verify information accuracy.

Document Layout

Research transition activities are addressed in four categories: collaborations, student research, communication products, and research transfers. In addition, there are sections covering topical workshops, news articles, and fact sheets. The research transition activities are listed by project and include project number, title, and the name of the principal investigator.

1. *Collaborations.* This section reports the collaborative effort being undertaken by EMSP projects to further research and to transfer research towards technical maturity. 42 collaborations have been reported. These are further categorized by type of collaboration, as follows:

Type of Collaboration	Number of each type
Consulting - provide advice or technical expertise	19
Joint interaction - researcher/end-user in joint interaction	6
Mission directed - project direction provided by end-user	6
Program interaction - researcher to researcher interaction	10
Unclassified	1

2. *Graduate Students.* One of the two main objectives of the EMSP is to develop a cadre of environmental scientists to meet 21st century clean-up needs. This

section tracks the impact the EMSP is having on increasing the cadre of environmental researchers. The number of Post Doctoral, PhD, Masters, and Undergraduate students are reported by EMSP project. Graduate student researcher's names are noted where provided. As of December 31, 1999, 474 undergraduate, graduate, and post graduate researchers were funded under this program.

3. *Publications and Presentations.* This section provides a list of publications by EMSP project. Journal articles, papers, reports, presentations, posters, and media reports are considered publications for the purposes of this summary. The following table lists the totals for each of these categories.

Type of Publication/Presentation	Number of each type
Journal Articles	329
Other (Encyclopedias, manuscripts)	39
Papers	55
Patent disclosures and applications	4
Posters	17
Presentations	368
Press Releases	5
Proceeding Contributions	98
Reports	35
Submitted for Consideration	133

4. *Research Transfers.* The main objective of EMSP-funded research is to address EM clean-up needs through 2070. This section includes research transfers (i.e., deployments, products, spin-off business, field tests, continuation by others, etc.) by project. Some activities listed in this section may be planned actions and are provided to ensure follow-up contacts are made.

Type of Research Transfer	Number for each type
Commercializations	6
Field Tests	6
Focus Areas & Crosscutting Programs	3
Patents	8
Processes - IPP	1
Products - Unknown	1

Collaborations

EMSP COLLABORATIONS

Research results are not always directly transferred to a specific end-user. Collaborations or interactions between EMSP researchers and others occur that increase the body of knowledge in a specific area as a direct result of EMSP funded research. This comes in many forms:

- 19 Consulting - provide advice or technical expertise
- 6 Joint interaction - researcher and end-user in joint interaction
- 6 Mission directed - project direction provided by end-user
- 10 Program interaction - researcher to researcher interaction
- 1 Unclassified.

This section describes the reported collaborations that have occurred within the EMSP. Numerous other less formal collaborations occur during the EMSP topical and national workshops. Many of these are anticipated to mature into the research partnerships and research transfers reported elsewhere in this document.

Project: 54506

Title: Acid-Base Behavior in Hydrothermal Processing of Wastes
PI: Dr. Keith P. Johnston *Institution:* University of Texas at Austin

Description: To develop this new branch of acid-base chemistry in water above 325?C and to achieve a breakthrough which could make hydrothermal oxidation a successful technology for the DOE, the objectives of this project are to develop a fundamental molecular understanding of the thermodynamics of ion solvation and acid-base equilibria and how they affect metal-ion complexation and salt solubility and to use this information to develop easily implemented, molecular-based models. Working with LANL on an experiment treating tank waste with high temperatures.
Collaboration Type: Joint interaction
Collaborator: Steve Buelow
Collaborating Organization: Los Alamos National Laboratory

Project: 54546

Title: Engineered Antibodies for Monitoring of Polynuclear Aromatic Hydrocarbons
PI: Dr. Alexander E. Karu *Institution:* University of California at Berkeley

Description: The objective of this project is to use molecular biological techniques to derive a set of antibodies with useful affinities and selectivities for recovery and detection of polynuclear aromatic hydrocarbons (PAHs) in environmental and biological samples. The long-term goal is to develop immunodetection methods that will be useful in biomarker research and regulatory monitoring of PAHs. Collaboration with Dr. Tuan Vo-Dinh at ORNL to identify sensor system and demonstration.
Collaboration Type: Mission directed
Collaborator: Dr. Tuan Vo-Dinh
Collaborating Organization: Oak Ridge National Laboratory

Project: 54656

Title: Mixing Processes in High-Level Waste Tanks
PI: Dr. Per F. Peterson *Institution:* University of California at Berkeley

Description: Flammable gases can be generated in DOE high-level waste tanks. This project is a concentrated effort to develop models and a numerical tool to mechanistically predict mixing processes in large waste-tank volumes, where mixing processes can be driven by hot and cold vertical and horizontal surfaces and injected buoyant jets. General Electric is funding a doctoral student to work on this project.
Collaboration Type: Consulting
Collaborator:
Collaborating Organization: General Electric

Project: 54672

Title: Radiation Effects in Nuclear Waste Materials
PI: Dr. William J. Weber *Institution:* Pacific Northwest National Laboratory

Description: Requested to assist in evaluating potential radiation-induced failure of protective glass globes for lights in the in-tank camera systems for Tank 101-SY at Hanford. Unexplained failure of two globes had raised some safety concerns. Working with Lockheed Martin Hanford Co. staff, an interim testing program was designed for the protective glass globes, a procedure to minimize potential failure (change globes frequently) was advised, and some preliminary measurements and evaluations were conducted on irradiated globes. No permanent solution was developed as yet.
Collaboration Type: Consulting
Collaborator: Scott M Werry
Collaborating Organization: Lockheed Martin Hanford Co.

Description: The effects of radiation from the decay of radionuclides in nuclear waste and other nuclear materials may potentially impact the long-term performance and stability of nuclear waste forms and stabilized nuclear materials. Using experimental and computer simulation approaches, this project endeavors to develop the underpinning science and models necessary to assess the effects of radiation on the performance of glasses and ceramics designed for the immobilization of high-level tank waste and stabilized nuclear materials. Collaborations with N.J. Hess, B.D. Begg, L.R. Corrales, H.L. Heinisch, and R.E. Williford at PNNL and with S.D. Conradson at LANL.
Collaboration Type: Program interaction
Collaborator: N.J. Hess, B.D. Begg, L.R. Corrales, H.L. Heinisch, and R.E. Williford; S.D. Conradson
Collaborating Organization: Pacific Northwest National Laboratory; Los Alamos National Laboratory

Project: 54679

Title: Architectural Design Criteria for F-Block Metal Ion Sequestering Agents
PI: Dr. Benjamin P. Hay *Institution:* Pacific Northwest National Laboratory

Description: Critical tasks in the cleanup of U.S. Department of Energy (DOE) sites include processing radioactive wastes for disposal in long-term storage, remediation/restoration of environmental sites resulting from radioactive contamination, and decontamination/decommissioning of nuclear facilities.Because the radioactive components, most of which are metals, are typically present in very low concentrations, it is desirable to remove them from the bulk of the contaminated source and concentrate them to minimize the volume of radioactive material destined for permanent subsurface disposal and thus minimize disposal costs. Over the past 50 years, much research has focused on the discovery of selective ligands for f-block metal separations; both neutral and ionic ligands have been examined. Despite past success in the discovery of ligands that exhibit some degree of specificity for the f-block metal ions, the ability to further control binding affinity and selectivity remains a significant challenge. The objective of this project is to provide the means to optimize ligand architecture for f-block metal recognition. Criteria for accurately selecting target ligands would result in a much more effective use of resources, thereby reducing the time and cost associated with metal-specific ligand development. Collaborations for each associated task are as follows:

Task: Synthesis and characterization of modified calixarene host molecules.

- Professor D. Max Roundhill, Department of Chemistry, Texas Tech University

Task: Crystal structure determinations.

- Professor Robin D. Rogers, Department of Chemistry, The University of Alabama

Task: Synthesis of amides and diamides, through a subcontract with Associated Western Universities to support a Postdoctoral Fellow, Dr. Robert Gilbertson, In Dr. Hutchison's group.

- Professor James E. Hutchison, Department of Chemistry, University of Oregon

Task: Provide structure-function data on catecholates and hydroxypyridonates.

- Professor Kenneth N. Raymond, Department of Chemistry, University of California at Berkeley

Task: Provide structure-function data on pyridine N-oxides.

- Professor Robert T. Paine, Department of Chemistry, University of New Mexico

In addition to interactions with University faculty, the project has supported a variety of visitors at Pacific Northwest National Laboratory through Associated Western Universities subcontracts, including:

- Dr. Pier L. Zanonato (Visiting Faculty, University of Padova, Italy) - calorimetry
- Dr. Bruce K. McNamara (Postdoctoral Fellow) - calorimetry, spectroscopy, solventextraction
- Dr. Omoshile Clement (Postdoctoral Fellow) - molecular mechanics
- Dr. Giovanni Sandrone (Postdoctoral Fellow) - quantum mechanics
- Dr. Rubicelia Vargas (Post Doctoral Fellow) - molecular mechanics and quantummechanics
- Dr. Jorge Garza (Visiting Faculty, Metropolitan Autonomous University -Iztapalapa, Mexico) - quantum mechanics

Collaboration Type: Program interaction
Collaborator: (see description)
Collaborating Organization: (See description)

Project: 54684

Title: Mechanism Involved in Trichloroethylene-Induced Liver Cancer: Importance to Environmental Cleanup
PI: Dr. Richard J. Bull *Institution:* Pacific Northwest National Laboratory

Description: EPA is using the data we have generated and a paper describing the mode of action for induction of liver tumors to revise their risk assessment on trichloroethylene. EPA continues to track our published results as this decision process reaches its conclusions. A separate step will be actions taken under the Office of Water to revise drinking water standards or CERCLA to modify clean-up standards that are derived from the revised risk assessments.
Collaboration Type: Consulting
Collaborator:
Collaborating Organization: EPA

Project: 54741

Title: Characterization of Contaminant Transport Using Naturally-Occurring U-Series Disequilibria
PI: Dr. Michael T. Murrell *Institution:* Los Alamos National Laboratory

Description: Consulted regarding uranium measurements at Rocky Flats by contractors for Rocky Flats and for the State of Colorado. We later received a small amount of funding to make some measurements for solar pond waters at Rocky Flats. The approach used was similar to that of our EMSP project.
Collaboration Type: Consulting
Collaborator: Dave Janecky
Collaborating Organization: Rocky Flats Environmental Technology Site, State of Colorado

Project: 54751

Title: High Fluence Neutron Source for Nondestructive Characterization of Nuclear Waste
PI: Dr. Mark M. Pickrell
Institution: Los Alamos National Laboratory

Description: The objective of the project is to research the basic plasma physics necessary to develop a high fluence neutron source based on the inertial electrostatically confined (IEC) plasma. An intense neutron source directly addresses the capability to characterize nuclear materials under difficult measurement conditions. Some of the applications for Environmental Management are the characterization of TRU wastes for WIPP, the measurements of residues prior to stabilization and disposal, the measurements of cemented or vitrified wastes, the measurement of spent nuclear fuel, and the measurement of high level wastes. Collaborations with the INEEL and the National Spent Nuclear Fuels Program to produce a neutron source for MDAS or other systems being developed by the INEEL.

Two commercial partners have applied for a license for the High Fluence Neutron Source, shown here in the laboratory. [see Project #54751]

Collaboration Type: Mission directed
Collaborator: Jerry Cole
Collaborating Organization: Idaho National Engineering and Environmental Laboratory

Project: 54828

Title: Processing of High Level Waste: Spectroscopic Characterization of Redox Reactions in Supercritical Water
PI: Dr. Charles A. Arrington, Jr. *Institution:* Furman University

Description: Collaborative research effort with LANL on the destructions of complexants and oxidation of chromium and technetium by hydrothermal processing in near critical or supercritical aqueous solutions.
Collaboration Type: Program interaction
Collaborator: Steven Buelow and Jeanne Robinson
Collaborating Organization: Los Alamos National Laboratory

Project: 54996

Title: Ionizing Radiation Induced Catalysis on Metal Oxide Particles
PI: Dr. Michael A. Henderson *Institution:* Pacific Northwest National Laboratory

Description: This project focuses on a novel approach for destroying organics found in high-level mixed waste prevalent at DOE sites. We have shown that ionizing radiation can be used to catalytically destroy organic chelating agents, such as EDTA, whose presence in high-level waste streams hinder the removal of radionucleii by ion exchange. Our studies have shown that gamma irradiation of titanium dioxide suspensions destroy the chelating ability of EDTA by decomposing it to smaller organic molecules. This has been demonstrated for both free EDTA in solution and for solutions of EDTA complexed to strontium. Present efforts are aimed at determining the mechanism by which EDTA is destroyed and the feasibility of using this process for treating high-level mixed waste.
Collaboration Type: Consulting
Collaborator: Abhaya K. Datye; Professor Miguel E. Castro
Collaborating Organization: University of New Mexico; University of Puerto Rico

Project: 55103

Title: Utilization of Kinetic Isotope Effects for the Concentration of Tritium
PI: Dr. Gilbert M. Brown *Institution:* Oak Ridge National Laboratory

Description: The objective of our work is to develop an electrochemically-based, cyclic process which can be used to remove tritium from contaminated water. We are developing methods for concentrating tritium from water based on large primary kinetic isotope effects in catalytic redox processes. H-T discrimination occurs in an oxidation step involving a transition metal oxidant and small organic compounds containing oxidizable C-H or C-T bonds. Tritium is incorporated in the organic compound by an electrochemical reduction process in the presence of tritium contaminated water, but the protio-derivative is kinetically favored in the oxidation half-reaction. As a result of a cyclic oxidation-reduction process, tritium is enriched in the organic compound. The organic compound is chosen so that it does not readily exchange the tritium with groundwater.
Collaboration Type: Consulting
Collaborator: C.H. Ho, Douglas J. Lemme, Leon Maya, and Frederick V. Sloop, Jr.; Poonam M. Narula and Thomas J. Meyer
Collaborating Organization: Oak Ridge National Laboratory; University of North Carolina at Chapel Hill

Project: 55110

Title: An Alternative Host Matrix Based on Iron Phosphate Glasses for the Vitrification of Specialized Nuclear Waste Forms
PI: Dr. Delbert E. Day *Institution:* University of Missouri-Rolla

Description: Certain high level wastes (HLWs) are not well suited for vitrification in borosilicate (BS) glasses because they contain components such as phosphates that are poorly soluble in a BS host matrix. The waste loading must be significantly reduced if one is to successfully vitrify such problematic wastes in a BS glass. Iron phosphate glasses offer a technically feasible and cost effective alternative to borosilicate glasses for vitrifying such HLWs. The main objective of the project was to investigate the atomic structure-property relationships, and glass forming and

crystallization characteristics, of these iron phosphate glasses and glasses containing nuclear waste components. Other physical properties such as density and thermal expansion were studied. Collaborations for each associated task are as follows:

Task: X-Ray Absorption Spectroscopy (EXANES/EXAFS) at the Stanford Synchrotron Radiation Laboratory

- Drs. David Shuh, Jerry Bucher, N.M. Edelstein, and Corwin Booth, Lawrence Berkeley National Laboratory
- Dr. Pat Allen, Lawrence Livermore National Laboratory

Task: Neutron and High Energy X-Ray Scattering

- Drs. Marie-Louise Saboungi, Yaspal Badyal, and Dean Heaffner, The Division of Materials Science, Intense Pulsed Neutron Source, and The Advanced Photon Source, Argonne National Laboratory

Task: Raman Spectroscopy

- Dr. Marcos Grimsditch, Division of Materials Science, Argonne National Laboratory
- Dr. Andrea Mogus-Milankovic, Ruder Boskovic Institute, Croatia

Task: Electron Spin Resonance Studies

- Dr. David Griscom, Naval Research Laboratory

Task: Electrical properties (conductivity, loss, and dielectric constant)

- Dr. Andrea Mogus-Milankovic, Ruder Boskovic Institute, Croatia

Collaboration Type: Program interaction
Collaborator: (see description)
Collaborating Organization: (see description)

Project: 55205

Title: A Fundamental Study of Laser-Induced Breakdown Spectroscopy Using Fiber Optics for Remote Measurements of Trace Metals
PI: Dr. Scott Goode *Institution:* University of South Carolina

Description: Improved technologies are required by DOE for characterization and monitoring for site clean-up and waste processing applications. Especially needed are field deployable methods and devices of real-time monitoring. Matrices of interest to the DOE are soils, slurries, and aqueous and non-aqueous solutions. Laser-induced breakdown spectroscopy (LIBS) is a useful method for determining the elemental composition of solids. The objective of this project is to determine the optimal excitation and collection conditions and sampling times for metal contaminants in different matrices, and an understanding of the strengths and limitations of using fiber optics for LIBS sampling. PI is in the process of establishing a collaboration with EMSL.
Collaboration Type: Unclassified
Collaborator:
Collaborating Organization: Environmental Molecular Sciences Laboratory

Project: 55229

Title: The No_x System in Nuclear Waste
PI: Dr. Dan Meisel *Institution:* University of Notre Dame

Description: This project, a collaborative ANL/PNNL effort, studies processes of the title system as it relates to the chemistry in high level liquid nuclear waste (HLW). The program is structured to transfer the information directly to the Hanford site operators (via "Organic Aging Studies, PI: Don Camaioni, PNNL). Our activity is also closely coordinated with another EMSP project ("Interfacial Radiolysis", PI: Thom Orlando, PNNL) and we include below our results that relate directly to that project. We determined the redox potential of the NO32- radical and its possible conversion to NO radical rather than to NO2. We also determined the redox potential of the analogous NO22- radicals because this parameter will determine whether such a conversion is possible. We concluded that both NO2 and NO radicals are important intermediates in HLW and the relative importance will depend on the concentration of nitrite in the waste tank. As a consequence we will coordinate our activity with a recently awarded EMSP project that focuses on NO chemistry and its derivatives ("Reactivity of Peroxynitrite", PI: Sergei Lymar, BNL).
Collaboration Type: Mission directed
Collaborator: Sergei Lymar, Thom Orlando
Collaborating Organization: BNL, Pacific Northwest National Laboratory

Project: 55264

Title: High Resolution Definition of Subsurface Heterogeneity for Understanding the Biodynamics of Natural Field Systems: Advancing the Ability for Scaling to Field Conditions
PI: Dr. Ernest L. Majer *Institution:* Lawrence Berkeley National Laboratory

Description: The objectives for this project were to develop and apply high-resolution seismic imaging methods for defining physical parameters (lithology, fracture content, fast paths, faults, etc.) that may be controlling flow and transport in naturally heterogeneous material. A primary aspect of the project was to determine if seismic imaging methods could resolve the details necessary to understand the physical heterogeneity controlling microbial behavior. Collaborations are with PNNL and INEEL. PNNL is collaborating in correlating the bacterial behavior to the zones of high permeability detected with the geophysics. INEEL provided the site (TAN) and drilling support as well as collaboration with other EMSP researchers (Colwell and Smith) in understanding the in-situ flow and microbial properties. There were also close collaborations with on site contractors (L. Peterson and T. Woods) in the collectionand processing of the data.
Collaboration Type: Consulting
Collaborator: Dr. Ardeth Simmons, LBL Yucca Mountain PM
Collaborating Organization: Yucca Mountain Project

Project: 55395

Title: Physics of DNAPL Migration and Remediation in the Presence of Heterogeneities

PI: Dr. Stephen H. Conrad *Institution:* Sandia National Laboratories

Description: For the Permanganate experiment, we worked with Dr. Jack Istok, a professor at Oregon State. Flushing with potassium permanganate has been investigated as an oxidizer that mineralizes TCE. Jack suspected that the manganese precipitate that forms as a mineralization product cause permeability reduction and thereby inhibit access between the TCE and the permanganate solution and this is precisely what we were able to visually observe in this experiment. The manganese precipitate formed a low permeability rind surrounding the DNAPL pools. Such results had not been seen previously, because for experiments run in uniform media, the DNAPL does not reside in pools. The permanganate oxidation process not likely to be as efficient as initially hoped in cases where DNAPL resides in pools. Perhaps intermittent flushes with a substance to dissolve away manganese precipitate might be possible.

Collaboration Type: Consulting
Collaborator: Dr. Jack Istok
Collaborating Organization: Oregon State

Description: The project involves conducting well-controlled laboratory experiments to better understand the physics of DNAPL migration and remediation in the presence of heterogeneities. The results will be used to test and to continue development of new modeling approaches. In addition, the results of the remediation experiments will be used to test the quantitative performance of remediation design codes within heterogeneous media. We intend to work closely with developers of each remediation approach to attempt to optimize the remedial process and show each technique in its best possible light. Towards that end, Alex Meyer, a professor at Michigan Tech, visited our lab and is collaborating with us on our first series of experiments looking at surfactant mobilization and solubilization of DNAPLs.

Collaboration Type: Consulting
Collaborator: Dr. Alex Meyer
Collaborating Organization: Michigan Tech

Description: For our MA surfactant experiment, we obtained surfactant advice from Alex Meyer and Lirong Zhong. The experiment used the surfactant MA and was designed to maximize solubilization while minimizing mobilization. Contrary to expectation, we observed dramatic mobilization. The DNAPL penetrated the aquitard and became inaccessible to the surfactant. Even though trapping number calculations predict some modest amount of mobilization, failure to account for DNAPL in pools resulted in significantly underestimating the potential for extensive downward mobilization. In observing the mobilization process, we discovered a previously unknown mobilization process that occurs when the surfactant front first encounters a pool. Very different interfacial tensions on either side of the surfactant front result in enhanced drainage of the DNAPL

pool. For our particular experimental conditions, due to downward mobilization and penetration of the DNAPL into fine-grained units, introduction of the MA surfactant actually made the problem worse.

Collaboration Type: Consulting
Collaborator: Dr. Alex Meyer and Lirong Zhiong
Collaborating Organization: Michigan Tech

Description: For the Tween surfactant experiment, we obtained surfactant advice from Dr. Kurt Pennell, a professor at Georgia Tech. We obtained much better results using the Tween surfactant. We observed only modest DNAPL mobilization because the Tween surfactant maintains a much higher water/organic interfacial tension. We also observed good solubilization. Complete cleanup was achieved after several pore volumes of flushing. Time lapse animation of this experiment yielded important insights into remediation process.

Collaboration Type: Consulting
Collaborator: Dr. Kurt Pennell
Collaborating Organization: Georgia Tech

Description: We worked with Dr. Varadarajan Dwarakanath of Duke Engineering to design the tracer test. It occurred to us that the certain conditions provided by our remediation experiments – subsequent to the emplacement if the DNAPL and prior to beginning the remediation – were ideal for performing a tracer test while requiring very little extra work. Partitioning tracer tests are designed to compare the breakthrough of partitioning and non partitioning tracers. Retardation of the tracers that partition into the organic phase provides a means to calculate the mass of DNAPL contained in the region swept by the tracer test. We found that the test worked qualitatively, indicating the presence of DNAPL, but the calculations significantly underestimated the mass of DNAPL in the chamber. We believe that failure to account for the fact that the vast majority of the DNAPL mass existed in large pools resulted in under-prediction of DNAPL mass. When significant DNAPL mass exists in pools, typical tracer flow rates do not allow sufficient time for partitioning/diffusion of the tracers into and out of large pools.

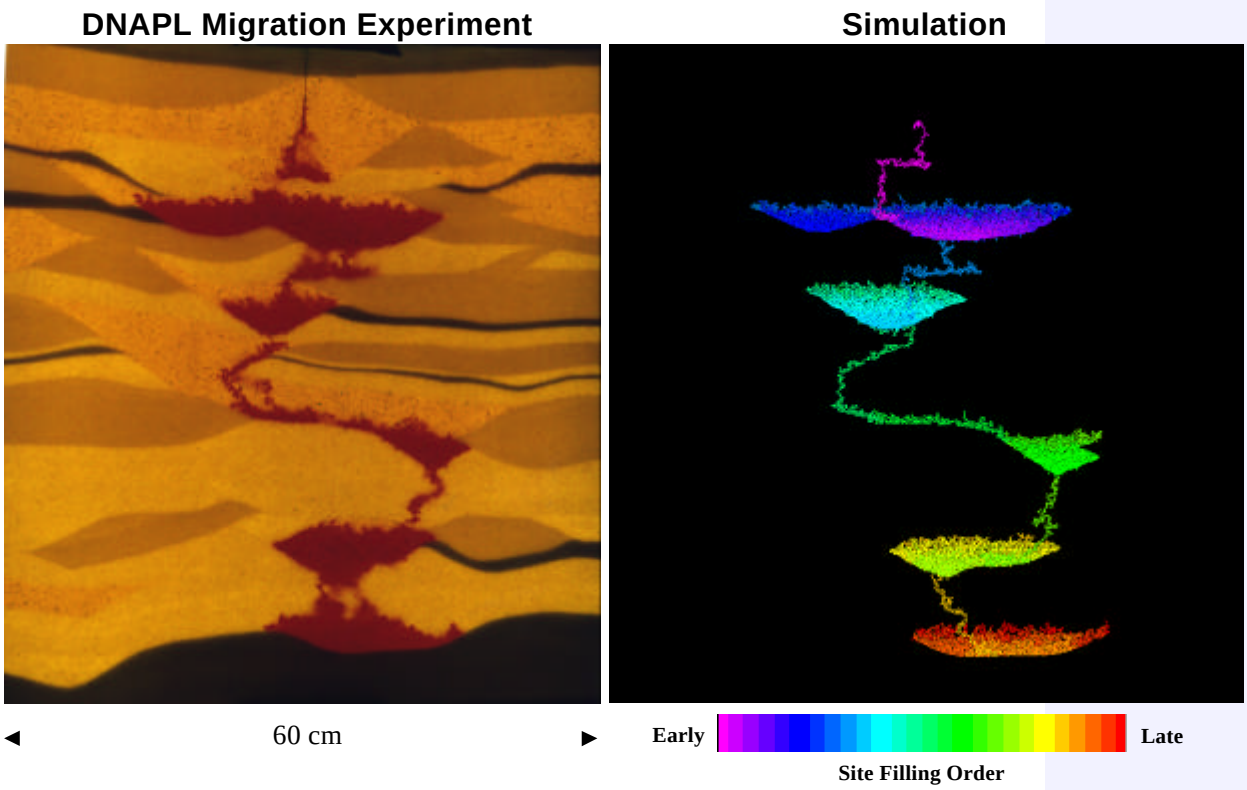
Collaboration Type: Consulting
Collaborator: Dr. Varadarajan Dwarakanath
Collaborating Organization: Duke Engineering

Project: 55410

Title: Determining Significant Endpoints for Ecological Risk Analysis
PI: Dr. Thomas G. Hinton *Institution:* Savannah River Ecology Laboratory

Description: The PI has taken knowledge gained from this research and used it in his work with the DOE Biota Dose Assessment Group (BDAG). BDAG is currently reviewing ecological risk concepts and establishing guidelines for conducting ecological risks on DOE Facilities.

Collaboration Type: Consulting
Collaborator: Dr. Thomas Hinton
Collaborating Organization: Savannah River Ecology Lab - University of Georgia



Results of a DNAPL migration experiment conducted at Sandia National Laboratories are compared to upscaled percolation modeling. The photo (left) illustrates that the DNAPL(dyed red) migrated downward due to its high density but that aquifer heterogeneities caused significant pooling along the migration path. DNAPL in such a configuration served as the initial condition for remediation experiments. The simulation image (right) compares extremely well with the experiment. [see Project #55395]

Project: 55416

Title: Control of Biologically Active Degradation Zones by Vertical Heterogeneity: Applications in Fractured Media

PI: Dr. Frederick S. Colwell *Institution:* Idaho National Engineering and Environmental

Description: The DOE is faced with cleaning up wastes from reactor and weapons production activities during the last fifty years. Many DOE sites have contaminants that are difficult to access due to depth and complex geology and are challenging to degrade using conventional methods. The key objective of this project is to determine the distribution of biologically active contaminant degradation zones in a fractured, subsurface medium with respect to vertical heterogeneities.

Collaboration Type: Consulting

Collaborator: Lance Peterson, Kent Sorenson, and Joe Rothermel

Collaborating Organization: Idaho National Engineering and Environmental Laboratory; Parsons

Project: 59849

Title: Radionuclide Immobilization in the Phases Formed by Corrosion of Spent Nuclear Fuel: The Long-Term Assessment
PI: Dr. Rodney C. Ewing *Institution:* University of Michigan

Description: Continued efforts to evaluate the capabilities of the uranyl phases to incorporate and retard release of important radionuclides: Np-237, Se-79, Tc-99, and I-129.
Collaboration Type: Program interaction
Collaborator: Professor Peter Burns
Collaborating Organization: Notre Dame

Project: 59882

Title: Measurements of Radon, Thoron, Isotopic Uranium and Thorium to Determine Occupational & Environmental Exposure & Risk at Fernald Feed Materials Production Center.
PI: Dr. Naomi H. Harley *Institution:* New York University Medical School

Description: Dr. Fisenne at USDOE Environmental Measurements Laboratory has developed a sequential radiochemical procedure to analyze any environmental sample matrix, presently focused on Soil samples, for Lead-210, radium, thorium, and uranium isotopes
Collaboration Type: Consulting
Collaborator: Dr. Isabel Fisenne
Collaborating Organization: Environmental Measurements Laboratory

Project: 59918

Title: Improved Radiation Dosimetry/Risk Estimates to Facilitate Environmental Management of Plutonium Contaminated Sites
PI: Dr. Bobby R. Scott *Institution:* Lovelace Biomedical & Environmental Research

Description: Additional data on lung cancer induced in Mayak workers exposed by inhalation to both plutonium and cigarette smoke were acquired by Dr. Scott from scientists at the Branch No. 1 of the Institute of Biophysics, Ozersk Russia. The data will facilitate making conclusions about possible interactions between alpha radiation and cigarette smoke in the induction of lung cancer. The data will also allow for additional insights to be made related to the validity of the linear, no-threshold hypothesis for cancer induction
Collaboration Type: Mission directed
Collaborator: Unknown
Collaborating Organization: Branch No. 1 of the Institute of Biophysics, Ozersk Russia

Description: We are now assisting staff at the Rocky Mountain Remediation Services, L.L.C., Rocky Flats Environmental Technology Site in preparing a scientifically valid approach to selecting respiratory protection devices for use in very high concentrations of plutonium. Some concentration of interest would essentially lead to early occurring or delayed deaths

without adequate worker protection. The activities at Rock Flats relate to decontamination and decommissioning. Our staff reviewed an original draft white paper related to selecting appropriate respiratory devices and major shortcomings related to protecting DOE decontamination/decommissioning workers were pointed out. We will continue to assist in preparing a more credible plan for protecting workers and in preparing an associated white paper

Collaboration Type: Consulting
Collaborator: Rocky Mountain Remediation Services, L.L.C.,
Collaborating Organization: Rocky Flats Environmental Technology Site

Project: 59960

Title: Direct Investigations of the Immobilization of Radionuclides in the Alteration Phases of Spent Nuclear Fuel
PI: Dr. Peter C. Burns *Institution:* University of Notre Dame

Description: The NSNFP is interested in this research concerning the mobility of the radionuclides in SNF for their work on the repository at Yucca Mtn. Dr. Burns is collaborating with ANL-E, where they are performing drip tests in a hot cell on commercial SNF. Ms. Davis has a work package funded by the NSNFP which funds ANL-E to perform similar release rate testing on DOE SNF. She is interested in having Dr. Burns perform an analysis on DOE SNF, similar to what he has done on commercial SNF. Dr. Paul Lessing is investigating the incorporation of Gadolinium as a neutron absorber into the DOE SNF packages which will be sent to Yucca Mtn. He would be interested in having Dr. Burns investigate the mobility of Gd in SNF packages.
Collaboration Type: Mission directed
Collaborator: Colleen Shelton-Davis
Collaborating Organization: National Spent Nuclear Fuels Program

Description: Solved the crystal structure of a novel uranyl silicate formed during the corrosion of an actinide-bearing waste glass.
Collaboration Type: Program interaction
Collaborator: Rudolph Olson
Collaborating Organization: Argonne National Laboratory

Project: 60020

Title: Stability of High-Level Waste Forms
PI: Dr. Theodore M. Besmann *Institution:* Oak Ridge National Laboratory

Description: Experimental studies of phase relations in the sodium oxide-boron oxide-uranium (VI) oxide system are being run in this EMSP program because there is no information in the literature. This data is needed for modeling actinide behavior in glasses. The results of these tests are also being spun off to assist the Uranium-233 Disposition Program of the Office of Fissile Materials Disposition (DOE/MD). They are considering dissolution of uranium oxide in sodium borate or boron oxide as an

option for Uranium-233 disposition. As experimental data is produced, it is made available to the Uranium-233 Program to assist in their development of a flow sheet. Because of the dearth of information on this system, it is not surprising that any information that is produced may be applied in different activities.

Collaboration Type: Joint interaction
Collaborator: Charles Forsberg
Collaborating Organization: Oak Ridge National Laboratory

Description: Models of phase relations and liquidus temperatures developed in this EMSP program are being used to evaluate test results from the Tanks Focus Area Immobilization Program "Waste Loading Improvements in High and Low Activity Glasses and Waste Form Product Acceptance Testing." The focus at this time is on conditions where crystallization occurs in glass processing. By applying models to the test data, an understanding of crystallization and how to avoid it may be obtained.

Collaboration Type: Joint interaction
Collaborator: John Vienna
Collaborating Organization: Pacific Northwest National Laboratory

Project: 60069

Title: Least-Cost Groundwater Remediation Design Using Uncertain Hydrogeological Information
PI: Dr. George F. Pinder *Institution:* University of Vermont

Description: The project seeks to examine the importance of uncertainty in hydraulic conductivity in the least-cost design of groundwater contamination containment systems. The project uses a new conceptual approach to accommodate aquifer parameter uncertainty in optimal groundwater remediation design and introduces a new operations-research technique to solve the optimization problem. The new approach, Robust Optimization, allows for the determination of a robust, lowest-possible cost, pumping design that is consistent with the inherent uncertainty in the hydraulic conductivity field. It also allows for the visualization of how one can trade off excess pumping for enhanced security. Collaborated with BNL for a review of Brookhaven groundwater contamination.

Collaboration Type: Consulting
Collaborator:
Collaborating Organization: Brookhaven National Laboratory

Project: 60075

Title: Particle Generation by Laser Ablation in Support of Chemical Analysis of High Level Mixed Waste from Plutonium Production Operations
PI: Dr. J. Thomas Dickinson *Institution:* Washington State University

Description: Performing laser ablation/description analytical determination on a surrogate sample. Contacted Arlin Olson and Scott Herbst to identify the surrogate and analytical requirements. Investigate analysis of these samples by laser ablation IMP-MS as well as a related method, laser desorption mass spectroscopy to determine key molecular components. The goal is to generate a complete mass balance of the calcine waste
Collaboration Type: Joint interaction
Collaborator: Jim Rindfleisch
Collaborating Organization: Long Range Waste Management Program, Idaho National Engineering and Enviornmental Laboratory

Description: We have been working with Dr. Beverly Crawford. Dr. Crawford is in charge of a laser ablation ICP-MS system that has been installed in a hot cell in the Hanford 222S building. One of the key technical questions is how well laser ablation can determine the overall bulk composition of a heterogeneous sample given a small volume of material sampled. We have begun to address the homogeneity issue .
Collaboration Type: Joint interaction
Collaborator: Dr. Beverly Crawford
Collaborating Organization: Numatec, Hanford

Project: 60118

Title: Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms
PI: Dr. Mark A. Williamson *Institution:* Los Alamos National Laboratory

Description: The end of the Cold War raised the need for the technical community to be concerned with the disposition of excess nuclear weapon material. The plutonium will either be converted into mixed-oxide fuel for use in nuclear reactors or immobilized in glass or ceramic waste forms and placed in a repository. The stability and behavior of plutonium in the ceramic materials as well as the phase behavior and stability of the ceramic material in the environment is not well established. The purpose of this project is to determine the thermodynamic data essential to developing an understanding of the chemistry and phase equilibria of the waste form materials proposed as immobilization matrices. Collaboration with DOE-MD program for Dispositioning of Plutonium by
Collaboration Type: Program interaction
Collaborator:
Collaborating Organization: DOE-Office of Fissile Materials Disposition

Project: 60283

Title: Waste Volume Reduction Using Surface Characterization and Decontamination by Laser Ablation

PI: Dr. Michael J. Pellin *Institution:* Argonne National Laboratory

Description: The waste stream generated in the D&D efforts for nuclear facilities includes a significant volume of material that is contaminated only in the surface or near-surface region. It is critical to understand the depth-dependent concentration and chemistry of radionuclide-contaminated surfaces. Complete removal and capture of the contaminated surface would greatly reduce the volume of waste material generated in, and thus the cost of, D&D efforts. This project represents the first detailed surface studies of the sorption of radionuclides in complex materials such as concrete. Collaboration is a joint interaction with Zawtech Inc. to do further research into areas of practical applications

Collaboration Type: Joint interaction

Collaborator:

Collaborating Organization: Zawtech Inc.

Project: 60296

Title: Research Program to Investigate the Fundamental Chemistry of Technetium

PI: Dr. Norman M. Edelstein *Institution:* Lawrence Berkeley National Laboratory

Description: This project addresses the fundamental solution chemistry of technetium (Tc) in the waste tank environment, and the stability of Tc in various waste forms. A separate facet of this project is the search for lower valent forms of Tc that may be incorporated in various waste forms for long term storage. Collaborated with PNNL as a participant (technical expert) at Technetium Chemistry workshop review panel assessing tank technetium removal/disposition options.

Collaboration Type: Consulting

Collaborator:

Collaborating Organization: Pacific Northwest National Laboratory

Project: 60362

Title: Ion-Exchange Processes and Mechanisms in Glasses

PI: Dr. B. Peter McGrail *Institution:* Pacific Northwest National Laboratory

Description: The objective of this project is to develop an understanding of the processes and mechanisms controlling alkali ion exchange and to correlate the kinetics of the ion-exchange reaction with glass structural properties. The fundamental understanding of the ion-exchange process developed under this study will provide a sound scientific basis for formulating low exchange rate glasses with higher waste loading, resulting in substantial production and disposal cost savings. Collaboration with Dr. David K. Shuh at the Lawrence Berkeley National Laboratory

Collaboration Type: Program interaction
Collaborator: D.K. Shuh
Collaborating Organization:

Project: 60403

Title: Phase Chemistry of Tank Sludge Residual Components
PI: Dr. James L. Krumhansl *Institution:* Sandia National Laboratories

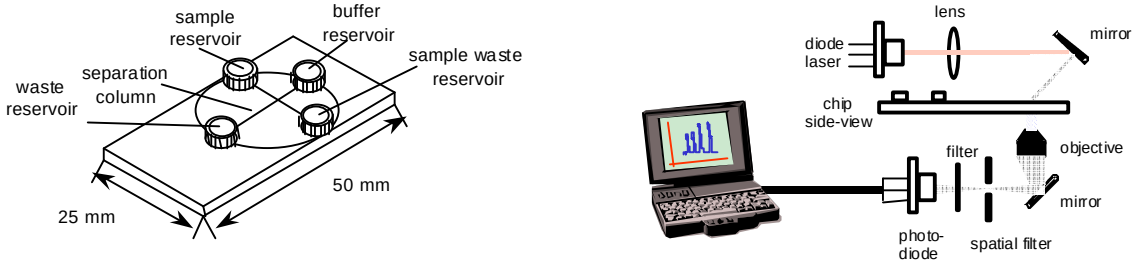
Description: Because it is not possible to recover all of the contaminated sludge from the bottoms of decommissioned waste storage tanks, a credible model for the release of radionuclides from residual sludge is needed. Those sludge components most likely to retain radionuclides will be identified and synthesized. Radionuclide sorption and desorption will also be studied. AFM and STM studies will provide a firm atomistic explanation for the observed interactions between the sludge, solutions, and radionuclides. This understanding will be used to develop a quantitative radionuclide release source term for use in the performance assessment calculations. Collaboration with Larry Bustard at TFA regarding aspects of tank fluid/sludge interactions.
Collaboration Type: Consulting
Collaborator: Larry Bustard
Collaborating Organization: TFA

Project: 64982

Title: Metal Ion Analysis Using Near-Infrared Dyes and the "Laboratory-on-a-Chip"
PI: Dr. Greg E. Collins *Institution:* Naval Research Laboratory

"Laboratory-on-a-Chip"

Instrumentation



J.M. Ramsey et. al., AnalChem, 67, 2059 (1995).

The Laboratory-on-a-Chip is intended to provide a field portable characterization instrument for in-situ waste characterization. [see Project #64982]

Description: This project addresses the need for developing a new class of radionuclide and heavy metal complexation agents that are tagged with near-infrared dyes and, therefore, can be extended to the implementation of a compact and portable "laboratory-on-a-chip" operable in the stringent field requirements of DOE site characterization and remediation. Collaboration with Dick Meservey with the Decontamination and Deactivation Focus Area to refine the project direction. Commitments to support field-testing have been

Collaboration Type: Mission directed
Collaborator: Dick Meservey
Collaborating Organization: DDFA

Project: 65411

Title: Precipitation and Deposition of Aluminum-Containing Phases in Tank Wastes
PI: Dr. Jun Liu *Institution:* Pacific Northwest National Laboratory

Description: Aluminum-containing phases represent the most prevalent solids that can appear or disappear during the processing of radioactive tank wastes. Of all constituents of tank waste, Al-species have the greatest potential for clogging pipes and transfer lines, fouling highly radioactive components such as ion exchangers, and completely shutting down processing operations. The primary focus of this project is to understand the major factors controlling precipitation, scale formation, and cementation of existing soluble particles by Al-containing phases. The results will be used to predict and control precipitation, scale formation, and cementation under tank waste processing conditions. The results will also provide information regarding what Al-containing phases form and how soluble such phases are in basic tank waste solutions. The project will have an important impact on waste minimization and on the retrieval, transport, and separation of tank wastes. Collaboration with Dr. Albert Hu at Lockheed Martin Hanford Company to perform simulations to support the ESP modeling work at Hanford.

Collaboration Type: Program interaction
Collaborator: Dr. Albert Hu
Collaborating Organization: Lockheed Martin Hanford Company

Project: 65435

Title: Millimeter-Wave Measurements of High Level and Low Activity Glass Melts
PI: Dr. Paul P. Woskov *Institution:* Massachusetts Institute of Technology

Description: The objectives of the project are to develop new real-time sensors for characterizing glass melts in high level waste (HLW) and low activity waste (LAW) melters, and to understand the scientific basis and bridge the gap between glass melt model data and melter performance. A basic goal is to characterize glass melts in-situ with the new diagnostic

capability so that data will represent the actual melt's behavior. The work will be closely coupled to the needs of the Defense Waste Processing Facility, West Valley Demonstration Project, and vitrification efforts at Hanford, Oakridge, and Idaho sites. The project is a collaboration between the MIT Plasma Science and Fusion Center, PNNL, and the Savannah River Technology Center. In addition, discussions are in progress with Tom Thomas of the Tanks Focus Area regarding the possibility of demonstrating with the TFA.

Collaboration Type: Program interaction
Collaborator: Tom Thomas
Collaborating Organization: Tanks Focus Area

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EMSP STUDENT RESEARCH

One goal of the EMSP is to serve as a stimulus to focus the nation's science infrastructure on critical national environmental management problems. One of the primary ways to accomplish this goal is to increase the cadre of scientific expertise available to focus on EM problems. By making opportunities available for Post Doctoral, PhD, Masters, and Undergraduate research on EMSP projects, the program achieves this goal. This section describes the EMSP's accomplishments in the area of undergraduate, graduate, and post-graduate research support.

Project: 54546

Title: Engineered Antibodies for Monitoring of Polynuclear Aromatic Hydrocarbons
PI: Dr. Alexander E. Karu *Institution:* University of California at Berkeley
Student Researchers: 5

Project: 54571

Title: Removal of Heavy Metals and Organic Contaminants from Aqueous Streams by Novel Filtration Methods
PI: Dr. Nelly M. Rodriguez *Institution:* Northeastern University
Student Researchers: 8

Project: 54576

Title: On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow
PI: Dr. William G. Gray *Institution:* University of Notre Dame
Student Researchers: 1

Project: 54585

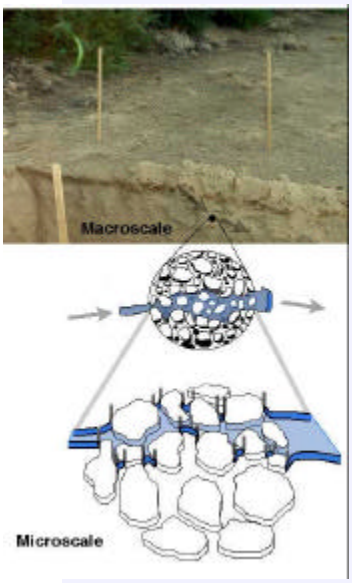
Title: Permanganate Treatment of DNAPLs in Reactive Barriers and Source Zone Flooding Schemes
PI: Dr. Frank W. Schwartz *Institution:* Ohio State University
Student Researchers: 3

Project: 54595

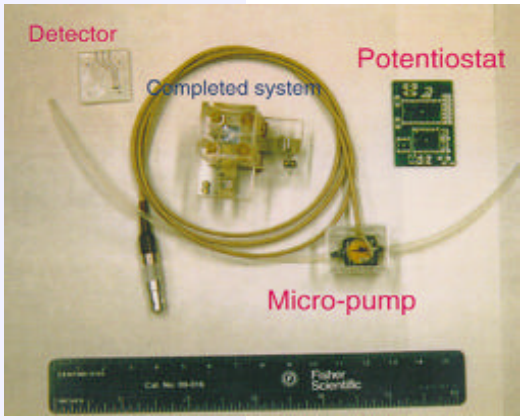
Title: f-Element Ion Chelation in Highly Basic Media
PI: Dr. Robert T. Paine *Institution:* University of New Mexico
Student Researchers: 3

Project: 54635

Title: Molecular-Level Process Governing the Interaction of Contaminants with Iron and Manganese
PI: Dr. Scott A. Chambers *Institution:* Pacific Northwest National Laboratory
Student Researchers: 10



The specific effects of interfacial behavior between interfaces that separate different fluids or separate fluids from solids is being more carefully studied so that their net impacts on fluid flow the macroscopic scale can be better understood. [see Project #54576]



NMSU / PNNL Electrochemical Metal Microanalyzer [see Project #54639]

Project: 54639

Title: Development of an In-Situ Microsensor for the Measurements of Chromium and Uranium in Groundwater at DOE Sites

PI: Dr. Joseph Wang

Institution: New Mexico State University

Student Researchers: 4

Project: 54656

Title: Mixing Processes in High-Level Waste Tanks

PI: Dr. Per F. Peterson

Institution: University of California at Berkeley

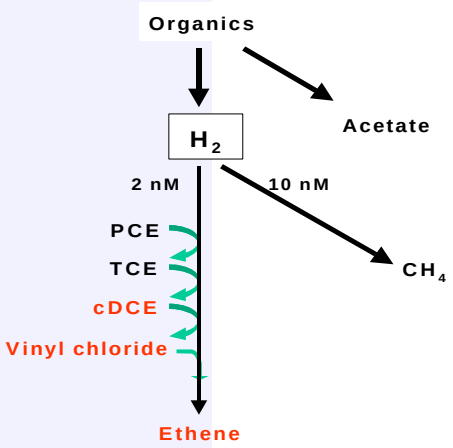
Student Researchers: 4

Project: 54661

Title: Electrochemical Processes for In-Situ Treatment of Contaminated Soils

PI: Dr. Chin-Pao Huang *Institution:* University of Delaware

Student Researchers: 1



PCE (or TCE) is stepwise reductively dehalogenated to the less chlorinated ethenes cDCE and VC. Concentration values indicate the hydrogen threshold concentration below which a pathway (dehalogenation or methanogenesis) usually does not operate. [see Project #54666]

Project: 54666

Title: Mechanisms, Chemistry, and Kinetics of Anaerobic Biodegradation of cDCE and Vinyl Chloride

PI: Dr. Perry L. McCarty

Institution: Stanford University

Student Researchers: 3

Project: 54672

Title: Radiation Effects in Nuclear Waste Materials

PI: Dr. William J. Weber

Institution: Pacific Northwest National Laboratory

Student Researchers: 2

Project: 54674

Title: Design and Development of a New Hybrid Spectroelectrochemical Sensor

PI: Dr. William R. Heineman

Institution: University of Cincinnati

Student Researchers: 18

Project: 54679

Title: Architectural Design Criteria for F-Block Metal Ion Sequestering Agents

PI: Dr. Benjamin P. Hay *Institution:* Pacific Northwest National Laboratory

Student Researchers: 2

Project: 54681

Title: Dynamics of Coupled Contaminant and Microbial Transport in Heterogeneous Porous Media

PI: Dr. Ellyn Murphy *Institution:* Pacific Northwest National Laboratory

Student Researchers: 2

Project: 54683

Title: Speciation and Structural Characterization of Plutonium and Actinide-Organic Complexes in Surface and Groundwaters

PI: Dr. Ken O. Buesseler *Institution:* Woods Hole Oceanographic Institute

Student Researchers: 1

Project: 54691

Title: Radiation Effects on Materials in the Near-Field of Nuclear Waste Repository

PI: Dr. Lu-Min Wang

Institution: University of Michigan

Student Researchers: 2

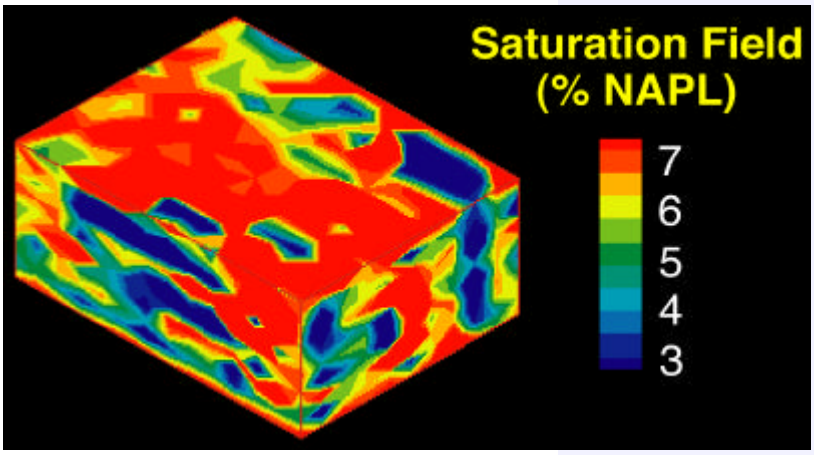
Project: 54716

Title: Polyoxometalates for Radioactive Waste Treatment

PI: Dr. Michael T. Pope

Institution: Georgetown University

Student Researchers: 4



NAPL saturation distribution estimated from partitioning tracer data for the Hill Air Force Base OU1 field test. [see Project #54716]

Project: 54724

Title: Synthesis of New Water-Soluble Metal-Binding Polymers: Combinatorial Chemistry Approach

PI: Dr. Barbara F. Smith

Institution: Los Alamos National Laboratory

Student Researchers: 4

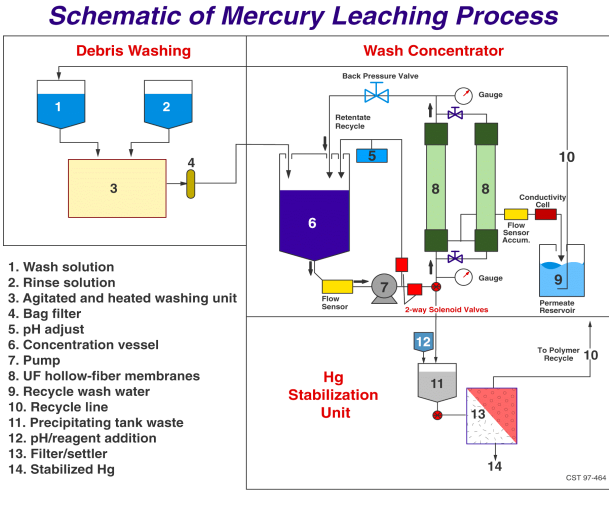
Project: 54735

Title: Development of Inorganic Ion Exchangers for Nuclear Waste Remediation

PI: Dr. Abraham Clearfield

Institution: Texas A&M University

Student Researchers: 12



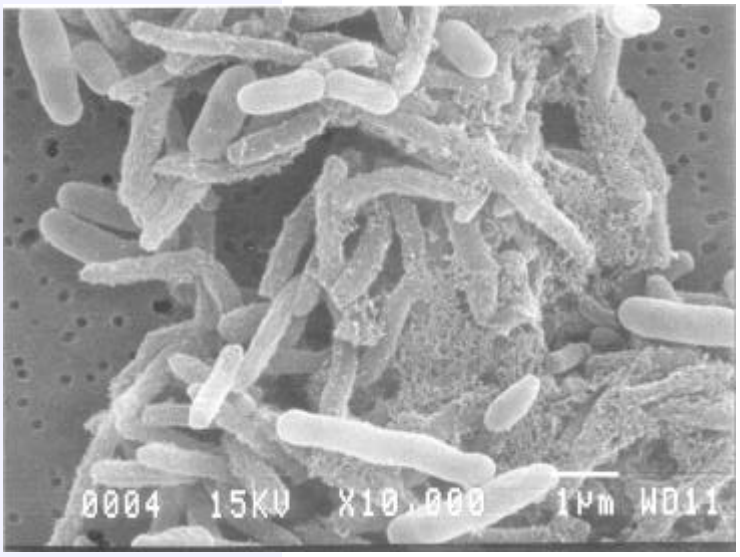
Schematic of Groundwater and Soil Remediation Process [see Project #54724]

Project: 54765

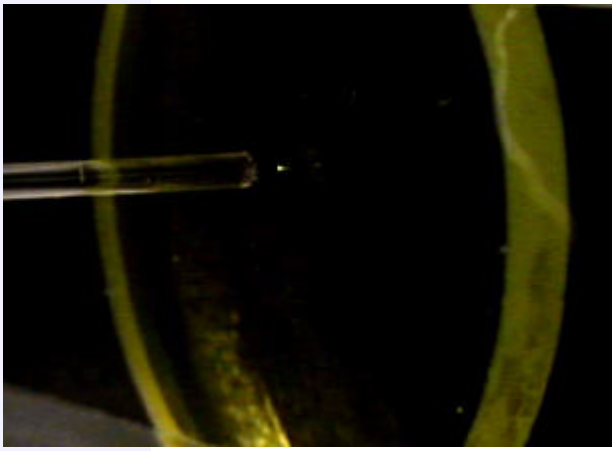
Title: Enhanced Sludge Processing of HLW: Hydrothermal Oxidation of Chromium, Technetium, and Complexants by Nitrate

PI: Dr. Stephen J. Buelow *Institution:* Los Alamos National Laboratory

Student Researchers: 7



A scanning electron microscope image showing dissimilatory iron-reducing bacteria with adherent hydrous ferric oxide. [see Project #54790]



An example of the capabilities of the Pacific Northwest Consortium beamline: A tapered glass capillary is used to produce a micron scale x-ray beam for microprobe applications. The micron size beam is visible as a glowing spot as it hits a scintillating screen. [see Project #54800]

Project: 54790

Title: Microbial Mineral Transformations at the Fe(II)/Fe(III) Redox Boundary for Solid Phase Capture of Strontium and Other Metal/Radionuclide Contaminants

PI: Dr. F. Grant Ferris

Institution: University of Toronto

Student Researchers: 6

Project: 54791

Title: Managing Tight-binding Receptors for New Separations Technologies

PI: Dr. Daryle H. Busch

Institution: University of Kansas

Student Researchers: 7

Project: 54793

Title: Establishing a Quantitative Functional Relationship Between Capillary Pressure, Saturation and Interfacial Area

PI: Dr. Carlo D. Montemagno

Institution: Cornell University

Student Researchers: 7

Project: 54800

Title: Construction of Bending Magnet Beamline at the APS for Environmental Studies

PI: Dr. Edward A. Stern

Institution: University of Washington

Student Researchers: 2

Project: 54807

Title: Studies Related to Chemical Mechanisms of Gas Formation in Hanford High-Level Nuclear Wastes

PI: Dr. E. Kent Barefield

Institution: Georgia Institute of Technology

Student Researchers: 3

Project: 54828

Title: Processing of High Level Waste: Spectroscopic Characterization of Redox Reactions in Supercritical Water

PI: Dr. Charles A. Arrington, Jr. *Institution:* Furman University

Student Researchers: 6

Project: 54856

Title: Structural Biology of the Sequestration & Transport of Heavy Metal Toxins: NMR Structure Determination of Proteins Containing the Cys-X-Y-Cys-metal Binding Motifs

PI: Dr. Stanley J. Opella *Institution:* University of Pennsylvania

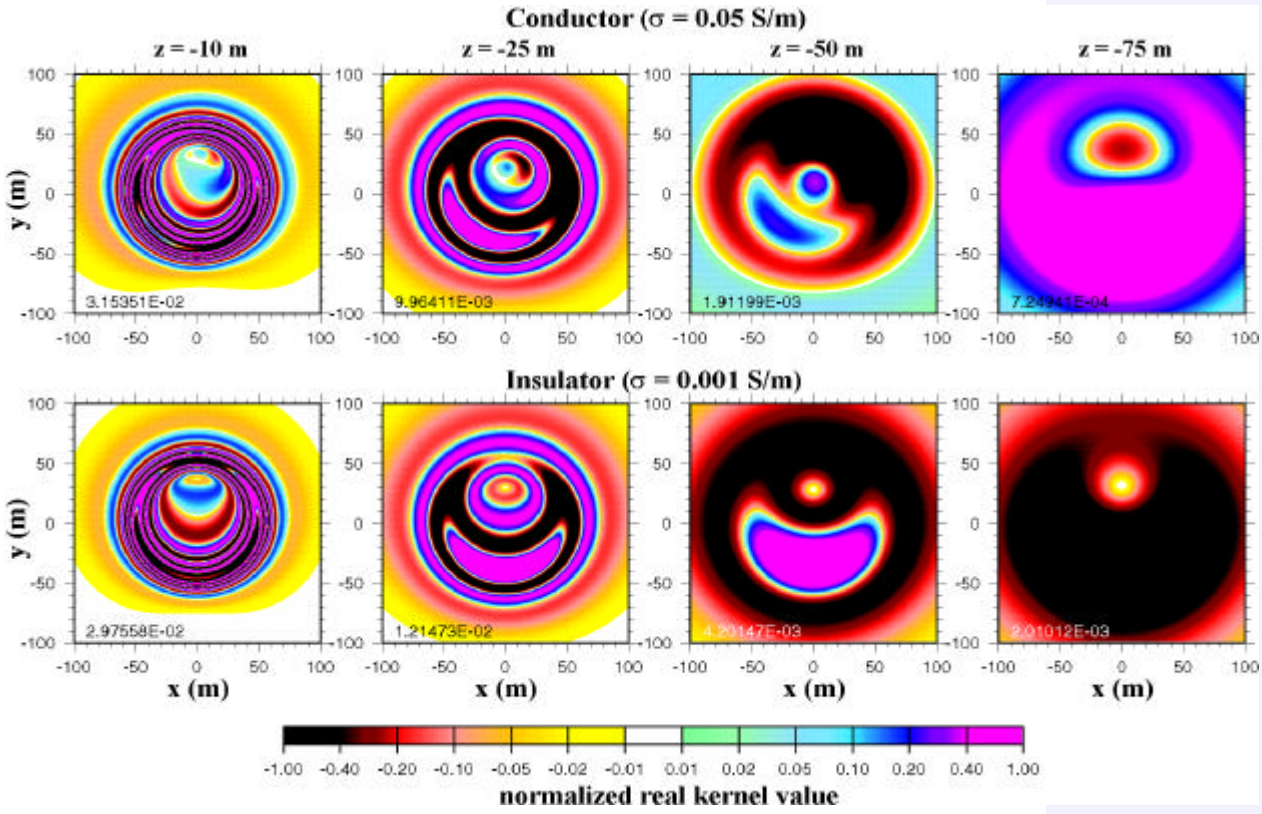
Student Researchers: 7

Project: 54857

Title: Surface Nuclear Magnetic Resonance Imaging of Water Content Distribution in the Subsurface

PI: Dr. Jan M.H. Hendrickx *Institution:* New Mexico Institute of Mining & Technology

Student Researchers: 2



The observed Nuclear Magnetic Resonance (NMR) response voltage response is given by the integration of an NMR sensitivity kernel against the free proton density function that characterizes the 3D water distribution. This figure shows horizontal (x-y) slices of the real part of the NMR sensitivity kernel at different specified depths (-10m, -25m, -50m, -75m) for a high resistivity (insulator) and low resistivity (conductive) half-space. This study derived for the first time the correct form of the kernels for a conducting medium. [see Project #54857]

Project: 54864

Title: Supramolecular Chemistry of Selective Anion Recognition for Anions of Environmental Relevance

PI: Dr. Kristin Bowman-James *Institution:* University of Kansas

Student Researchers: 11

Project: 54889

Title: Using Trees to Remediate Groundwaters Contaminated with Chlorinated Hydrocarbons

PI: Dr. Stuart E. Strand *Institution:* University of Washington

Student Researchers: 3

Project: 54897

Title: The Sonophysics and Sonochemistry of Liquid Waste Quantification and Remediation

PI: Dr. Thomas J. Matula *Institution:* University of Washington

Student Researchers: 2

Project: 54898

Title: Molecular Dissection of the Cellular Mechanisms Involved in Nickel Hyperaccumulation in Plants

PI: Dr. David E. Salt *Institution:* Northern Arizona University

Student Researchers: 5

Project: 54908

Title: Partitioning Tracers for In Situ Detection and Quantification of Dense Non-aqueous Phase Liquids in Groundwater Systems

PI: Dr. Mark L. Brusseau *Institution:* University of Arizona

Student Researchers: 7

Project: 54914

Title: Atmospheric-Pressure Plasma Cleaning of Contaminated Surfaces

PI: Dr. Robert F. Hicks *Institution:* University of California at Los Angeles

Student Researchers: 5

Project: 54926

Title: Novel Ceramic-Polymer Composite Membranes for the Separation of Hazardous Liquid Waste

PI: Dr. Yoram Cohen *Institution:* University of California at Los Angeles

Student Researchers: 7

Project: 54942

Title: Spectroscopy, Modeling and Computation of Metal Chelate Solubility in Supercritical CO_2

PI: Dr. Joan F. Brennecke *Institution:* University of Notre Dame

Student Researchers: 5

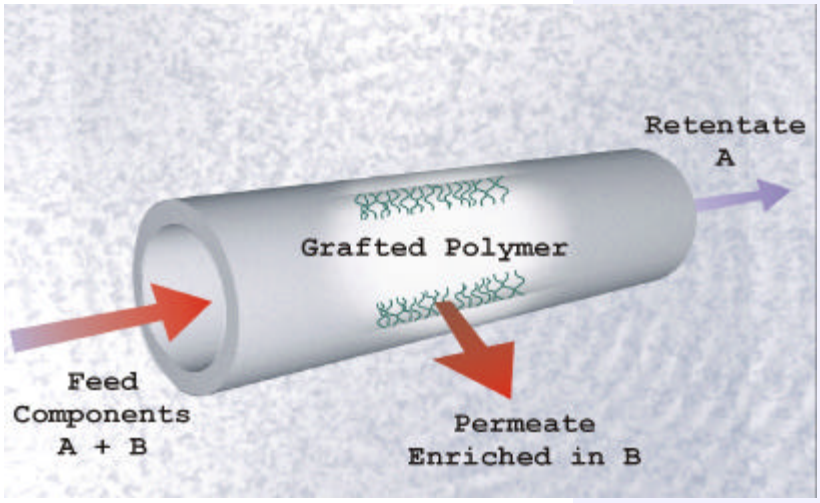
Project: 54973

Title: A Novel Energy-Efficient Plasma Chemical Process for the Destruction of Volatile Toxic

PI: Dr. Lal A. Pinnaduwage

Institution: Oak Ridge National Laboratory

Student Researchers: 3



Ceramic-Supported Polymer (CSP) Membranes [see Project #54926]

Project: 54982

Title: Analysis of Surface Leaching Processes in Vitrified High-Level Nuclear Wastes Using In-Situ Raman Imaging and Atomistic Modeling

PI: Dr. Joseph H. Simmons *Institution:* University of Florida

Student Researchers: 4

Project: 55012

Title: Extraction and Recovery of Mercury and Lead from Aqueous Waste Streams Using Redox-Active Layered Metal Chalcogenides

PI: Dr. Peter K. Dorhout *Institution:* Colorado State University

Student Researchers: 9

Project: 55013

Title: Biofiltration of Volatile Pollutants: Engineering Mechanisms for Improved Design, Long-term Operation, Prediction and Implementation

PI: Dr. Brian H. Davison

Institution: Oak Ridge National Laboratory

Student Researchers: 1

Project: 55014

Title: Kinetics and Mechanisms of Metal Retention/Release in Geochemical Processes in Soil

PI: Dr. Robert W. Taylor

Institution: Alabama A&M University

Student Researchers: 16

Metal Retention/Release Mechanisms for Geochemical Soil Processing. [see Project #55014]

Project: 55032

Title: Environmental Analysis of Endocrine Disrupting Effects from Hydrocarbon Contaminants in the Ecosystem

PI: Dr. John A. McLachlan

Institution: Tulane University

Student Researchers: 6

Project: 55033

Title: Characterization of Chemically Modified Hyperthermophilic Enzymes for Chemical Syntheses and Bioremediation Reactions

PI: Dr. Brian H. Davison *Institution:* Oak Ridge National Laboratory

Student Researchers: 2

Project: 55042

Title: Quantifying Silica Reactivity in Subsurface Environments: Controls of Reaction Affinity and Solute Matrix on Quartz and SiO_2 Glass Dissolution Kinetics

PI: Dr. Patricia M. Dove *Institution:* Georgia Institute of Technology

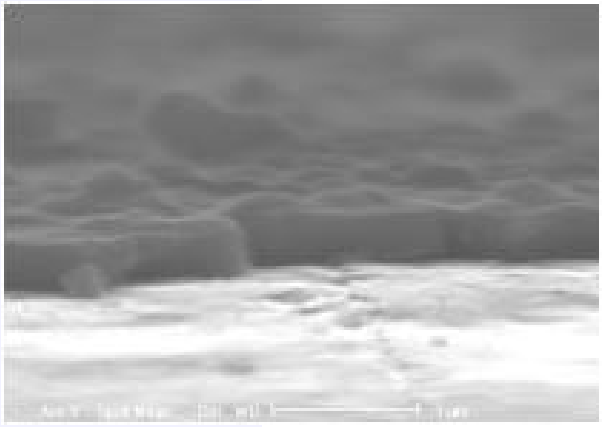
Student Researchers: 6

Project: 55052

Title: Advanced Sensing and Control Techniques to Facilitate Semi-Autonomous Decommissioning

PI: Dr. Robert J. Schalkoff *Institution:* Clemson University

Student Researchers: 14



Scanning Electron Microscope (SEM) image of an approximately 1 µm thick uranium oxide film grown atop an iron substrate by immersion under controlled conditions into a solution containing uranyl ions. This illustrates how iron can be used for the remediation of uranium dissolved in groundwater. [see Project #55061]

Project: 55061

Title: Fundamental Studies of the Removal of Contaminants from Ground and Waste Waters via Reduction by Zero-Valent Metals

PI: Dr. Jory A. Yarmoff

Institution: University of California at Riverside

Student Researchers: 6

Project: 55083

Title: Behavior of Dense, Immiscible Solvents in Fractured Clay-Rich Soils

PI: Dr. Larry D. McKay

Institution: University of Tennessee at Knoxville

Student Researchers: 4

Project: 55094

Title: Chemical and Ceramic Methods Toward Safe Storage of Actinides Using Monazite

PI: Dr. P. E. D. Morgan

Institution: Rockwell International Corporation

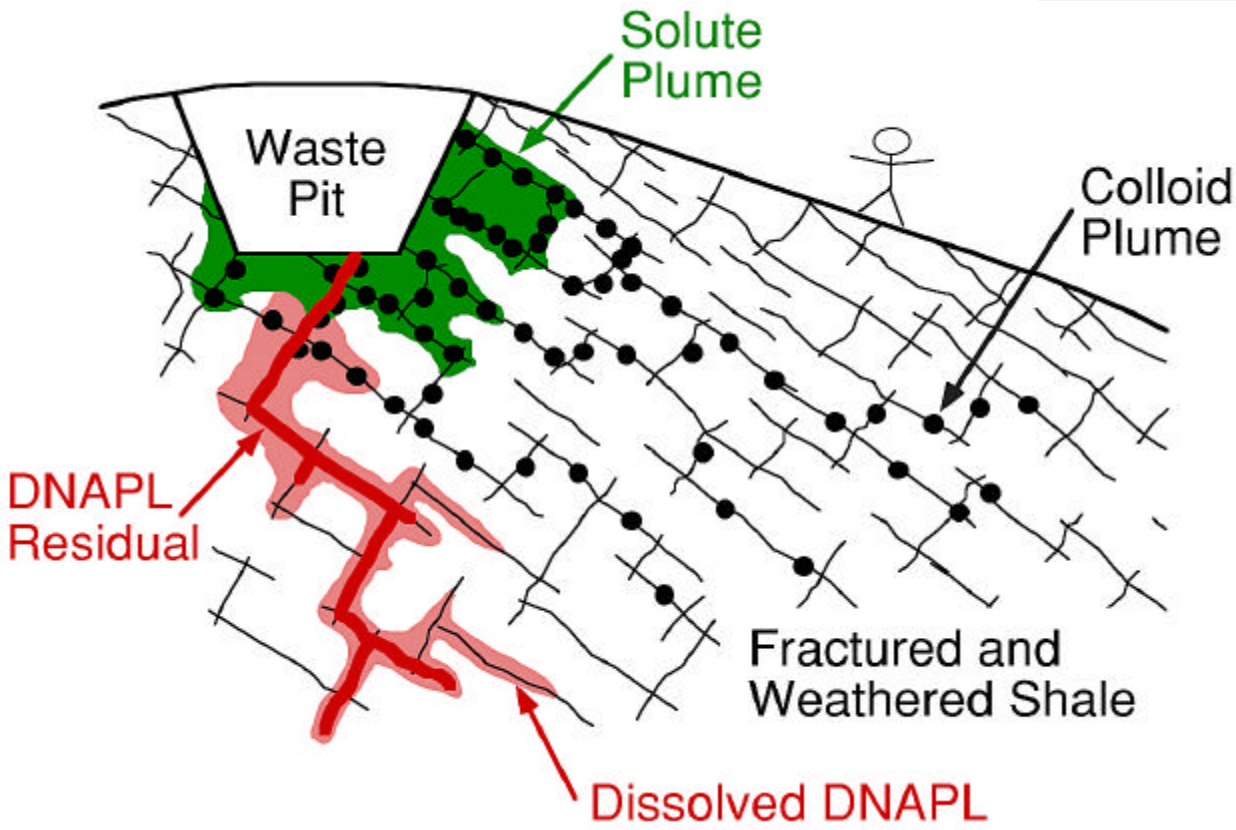
Student Researchers: 2

Project: 55097

Title: Heavy Metal Pumps in Plants

PI: Dr. Jeffrey F. Harper *Institution:* Scripps Research Institute

Student Researchers: 1



Migration of different contaminant types in fractured shales at Oak Ridge National Laboratory. Colloids migrate fastest, up to 200 m/day, because they are largely confined to fast-flow pathways in the fractures. Solutes, such as tritium, are strongly retarded relative to colloids because of diffusion into the relatively immobile pore water in the fine-grained matrix between fractures. DNAPLs can rapidly infiltrate downwards through the fractures, and then slowly dissolve forming plumes in the fractures and matrix pores. [see Project #55083]

Project: 55100

Title: Human Genetic Marker for Resistance to Radiations and Chemicals

PI: Dr. Howard B. Lieberman *Institution:* Columbia University

Student Researchers: 1

Project: 55108

Title: Monitoring Genetic & Metabolic Potential for In Situ Bioremediation: Mass Spectrometry

PI: Dr. Michelle V. Buchanan *Institution:* Oak Ridge National Laboratory

Student Researchers: 3

Project: 55110

Title: An Alternative Host Matrix Based on Iron Phosphate Glasses for the Vitrification of Specialized Nuclear Waste Forms

PI: Dr. Delbert E. Day *Institution:* University of Missouri-Rolla

Student Researchers: 3

Project: 55115

Title: The Adsorption and Reaction of Halogenated Volatile Organic Compounds (VOCs) on Metal Oxides

PI: Dr. Jack Lunsford *Institution:* Texas A&M University

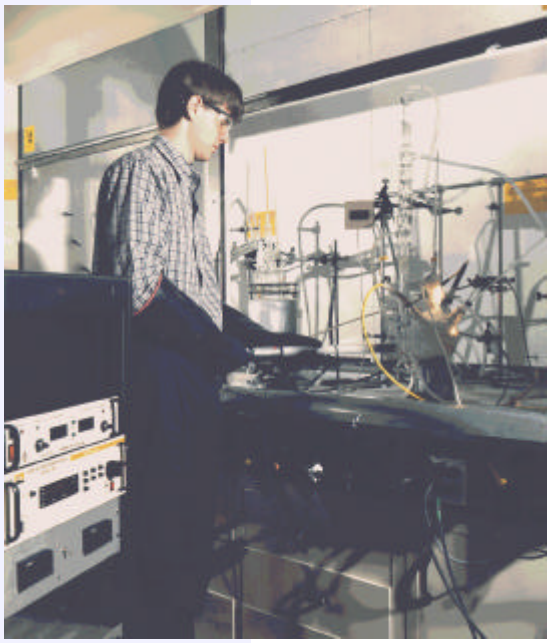
Student Researchers: 4

Project: 55118

Title: Plant Rhizosphere Effects on Metal Mobilization and Transport

PI: Dr. Teresa W. M. Fan *Institution:* University of California at Davis

Student Researchers: 2



Phase equilibria and interfacial transport may be modified to enhance separations by applying an electric field. A vapor-liquid-equilibrium experiment is shown here. [see Project #55119]

Project: 55119

Title: Phase Equilibria Modification by Electric Fields

PI: Dr. Costas Tsouris

Institution: Oak Ridge National Laboratory

Student Researchers: 1

Project: 55137

Title: Investigation of Novel Electrode Materials for Electrochemically-Based Remediation of High- and Low-Level Mixed Wastes in the DOE Complex

PI: Dr. Nathan S. Lewis

Institution: California Institute of Technology

Student Researchers: 8

Project: 55146

Title: Adsorption/Membrane Filtration as a Contaminant Concentration and Separation Process for Mixed Wastes and Tank Wastes

PI: Dr. Mark M. Benjamin

Institution: University of Washington

Student Researchers: 6

Project: 55152

Title: Molecular Profiling of Microbial Communities from Contaminated Sources: Use of Subtractive Cloning Methods and rDNA Spacer Sequences

PI: Dr. Frank T. Robb *Institution:* University of Maryland at Baltimore

Student Researchers: 5

Project: 55196

Title: In Situ, Field Scale Evaluation of Surfactant Enhanced DNAPL Recovery Using a Single-Well, Push-Pull Test

PI: Dr. Jonathan D. Istok *Institution:* Oregon State University

Student Researchers: 3

Project: 55211

Title: Cavitational Hydrothermal Oxidation: A New Remediation Process
PI: Dr. Kenneth S. Suslick
Institution: University of Illinois at Urbana-Champaign
Student Researchers: 3

Project: 55218

Title: Seismic Surface-Wave Tomography of Waste Sites
PI: Dr. Timothy L. Long
Institution: Georgia Institute of Technology
Student Researchers: 6

Graduate students collaborate on a field-scale evaluation of Surfactant Enhanced DNAPL Recovery using a single-well, push-pull test. [see Project #55196]

Project: 55223

Title: De Novo Design of Ligands for Metal Separation
PI: Dr. Garland R. Marshall *Institution:* Washington University
Student Researchers: 2

Project: 55278

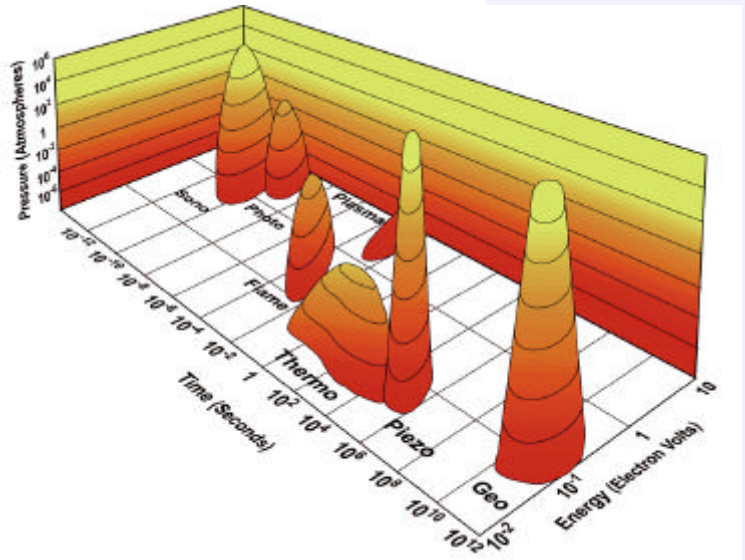
Title: Molecular Genetics of Metal Detoxification: Prospects for Phytoremediation
PI: Dr. David W. Ow
Institution: U.S. Dept. of Agriculture
Student Researchers: 1

Project: 55284

Title: Aquifer Transport of Th, U, Ra, and Rn in Solution and on Colloids
PI: Dr. G. J. Wasserburg
Institution: California Institute of Technology
Student Researchers: 2

Project: 55318

Title: Improved Analytical Characterization of Solid Waste Forms by Fundamental Development of Laser Ablation Technology
PI: Dr. Richard E. Russo
Institution: Lawrence Berkeley National Laboratory
Student Researchers: 3



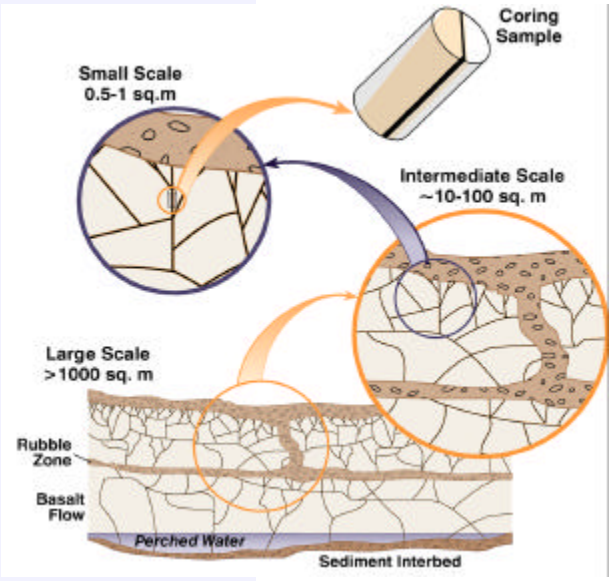
Chemical Islands. Chemistry is the interaction of energy and matter. The parameters that control this interaction are the amount of energy, the time of the interaction, and the pressure under which the interaction occurs. This describes the three dimensional space shown above, with many of the various types of chemistry shown in their proper place in this space. [see Project #55211]

Project: 55356

Title: Environmentally-Induced Malignancies: An In Vivo Model to Evaluate the Health Impact of Chemicals in Mixed Waste

PI: Dr. Maria Pallavicini *Institution:* University of California at San Francisco

Student Researchers: 2



A four-level hierarchy of scales of hydrogeological components in fractured basalt. [see Project #55359]

Project: 55359

Title: Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone

PI: Dr. Boris Faybishenko

Institution: Lawrence Berkeley National Laboratory

Student Researchers: 4

Project: 55374

Title: Use of Sonication for In-Well Softening of Semivolatile Organic Compounds

PI: Dr. Robert W. Peters

Institution: Argonne National Laboratory

Student Researchers: 2

Project: 55395

Title: Physics of DNAPL Migration and Remediation in the Presence of Heterogeneities

PI: Dr. Stephen H. Conrad

Institution: Sandia National Laboratories

Student Researchers: 3

Project: 55416

Title: Control of Biologically Active Degradation Zones by Vertical Heterogeneity: Applications in Fractured Media

PI: Dr. Frederick S. Colwell *Institution:* Idaho National Engineering and Environmental Laboratory

Student Researchers: 2

Project: 59786

Title: Design and Construction of *Deinococcus radiodurans* for Biodegradation of Organic Toxins at Radioactive DOE Waste Sites

PI: Dr. Michael J. Daly *Institution:* Uniformed Services Univ. of the Health Sciences

Student Researchers: 1

Project: 59827

Title: The Influence of Radiation and Multivalent Cation Additions on Phase Separation and Crystallization of Glass

PI: Dr. Michael C. Weinberg *Institution:* University of Arizona

Student Researchers: 3

Project: 59828

Title: Bioavailability of Organic Solvents in Soils: Input into Biologically Based Dose-Response Models for Human Risk Assessments

PI: Dr. Ronald C. Wester *Institution:* University of California at San Francisco

Student Researchers: 2

Project: 59918

Title: Improved Radiation Dosimetry/Risk Estimates to Facilitate Environmental Management of Plutonium Contaminated Sites

PI: Dr. Bobby R. Scott *Institution:* Lovelace Biomedical & Environmental Research

Student Researchers: 1

Project: 59925

Title: Modeling of Diffusion of Plutonium in Other Metals and of Gaseous Species in Plutonium-Based Systems

PI: Dr. Bernard R. Cooper *Institution:* West Virginia University

Student Researchers: 1

Project: 59934

Title: Hazardous Gas Production by Alpha Particles in Solid Organic Transuranic Waste Matrices

PI: Dr. Jay A. LaVerne *Institution:* University of Notre Dame

Student Researchers: 1

Project: 59960

Title: Direct Investigations of the Immobilization of Radionuclides in the Alteration Phases of Spent Nuclear Fuel

PI: Dr. Peter C. Burns *Institution:* University of Notre Dame

Student Researchers: 4

Project: 59977

Title: Synthesis and Characterization of Templated Ion Exchange Resins for the Selective Complexation of Actinide Ions

PI: Dr. George M. Murray *Institution:* Johns Hopkins University Applied Physics Lab

Student Researchers: 2

Project: 59990

Title: Fundamental Chemistry, Characterization, and Separation of Technetium Complexes in Hanford Waste

PI: Dr. Norman C. Schroeder *Institution:* Los Alamos National Laboratory

Student Researchers: 3

Project: 59993

Title: Dynamic Effects of Tank Waste Aging on Radionuclide-Complexant Interactions

PI: Dr. Rebecca Chamberlin *Institution:* Los Alamos National Laboratory

Student Researchers: 2

Project: 60015

Title: Long-term Risk from Actinides in the Environment: Modes of Mobility

PI: Dr. David D. Breshears *Institution:* Los Alamos National Laboratory

Student Researchers: 2

Project: 60017

Title: Removal of Technetium, Carbon Tetrachloride, and Metals from DOE Properties

PI: Dr. Thomas E. Mallouk *Institution:* Pennsylvania State University

Student Researchers: 3

Project: 60041

Title: Removal of Radioactive Cations and Anions from Polluted Water Using Ligand-Modified Colloid-Enhanced Ultrafiltration

PI: Dr. John F. Scamehorn *Institution:* University of Oklahoma

Student Researchers: 2

Project: 60069

Title: Least-Cost Groundwater Remediation Design Using Uncertain Hydrogeological Information

PI: Dr. George F. Pinder *Institution:* University of Vermont

Student Researchers: 2

Project: 60070

Title: The Development of Cavity Ringdown Spectroscopy as a Sensitive Continuous Emission Monitor for Metals

PI: Dr. George P. Miller *Institution:* Mississippi State University

Student Researchers: 2

Project: 60075

Title: Particle Generation by Laser Ablation in Support of Chemical Analysis of High Level Mixed Waste from Plutonium Production Operations

PI: Dr. J. Thomas Dickinson *Institution:* Washington State University

Student Researchers: 8

Project: 60096

Title: Rational Synthesis of Imprinted Organofunctional Sol-Gel Materials for Toxic Metal Separation

PI: Dr. Ziling Benjamin Xue *Institution:* University of Tennessee at Knoxville

Student Researchers: 9

Project: 60115

Title: Advanced High Resolution Seismic Imaging, Material Properties Estimation and Full Wavefield Inversion for the Shallow Subsurface
PI: Dr. Alan Levander *Institution:* Rice University
Student Researchers: 1

Project: 60118

Title: Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms
PI: Dr. Mark A. Williamson *Institution:* Los Alamos National Laboratory
Student Researchers: 3

Project: 60123

Title: Potential-Modulated Intercalation of Alkali Cations into Metal Hexacyanoferrate Coated
PI: Dr. Daniel T. Schwartz *Institution:* University of Washington
Student Researchers: 3

Project: 60143

Title: Foaming in Radioactive Waste Treatment and Immobilization Processes
PI: Dr. Darsh T. Wasan *Institution:* Illinois Institute of Technology
Student Researchers: 4

Project: 60144

Title: Flow Visualization of Forced and Natural Convection in Internal Cavities
PI: Dr. John C. Crepeau *Institution:* University of Idaho
Student Researchers: 4

Project: 60150

Title: Genetic Engineering of a Radiation-Resistant Bacterium for Biodegradation of Mixed Wastes
PI: Dr. Mary E. Lidstrom *Institution:* University of Washington
Student Researchers: 4

Project: 60158

Title: Development of Radon-222 as a Natural Tracer for Monitoring the Remediation of NAPL Contamination in the Subsurface
PI: Dr. Lewis Semprini *Institution:* Oregon State University
Student Researchers: 1

Project: 60163

Title: Investigation of Techniques to Improve Continuous Air Monitors Under Conditions of High Dust Loading in Environmental Settings
PI: Dr. Stephen D. Schery *Institution:* New Mexico Institute of Mining & Technology
Student Researchers: 1

Project: 60199

Title: Seismic-Reflection and Ground Penetrating Radar for Environmental Site Characterization

PI: Dr. Don W. Steeples *Institution:* University of Kansas

Student Researchers: 3

Project: 60218

Title: Novel Mass Spectrometry Mutation Screening for Contaminant Impact Analysis

PI: Dr. C. H. Winston Chen *Institution:* Oak Ridge National Laboratory

Student Researchers: 1

Project: 60219

Title: Development of Advanced Electrochemical Emission Spectroscopy for Monitoring Corrosion in Simulated DOE Liquid Waste

PI: Dr. Digby D. MacDonald *Institution:* Pennsylvania State University

Student Researchers: 1

Project: 60271

Title: Characterization of a New Family of Metal Transport Proteins

PI: Dr. Mary Lou Guerinot *Institution:* Dartmouth College

Student Researchers: 3

Project: 60326

Title: Isolation of Metals from Liquid Wastes: Reactive Scavenging in Turbulent Thermal Reactors

PI: Dr. Jost O. L. Wendt *Institution:* University of Arizona

Student Researchers: 9

Project: 60328

Title: High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification Efforts

PI: Dr. Ki-Ha Lee *Institution:* Lawrence Berkeley National Laboratory

Student Researchers: 1

Project: 60392

Title: Radiolytic and Thermal Process Relevant to Dry Storage of Spent Nuclear Fuels

PI: Dr. Steven C. Marschman *Institution:* Pacific Northwest National Laboratory

Student Researchers: 2

Project: 60401

Title: Mechanism of Pitting Corrosion Prevention By Nitrite in Carbon Steel Exposed to Dilute Salt Solutions

PI: Dr. Philip E. Zapp *Institution:* Westinghouse Savannah River Company

Student Researchers: 3

Project: 60451

Title: Mechanics of Bubbles in Sludges and Slurries
PI: Dr. Phillip A. Gauglitz *Institution:* Pacific Northwest National Laboratory
Student Researchers: 2

Project: 60474

Title: Ultrahigh Sensitivity Heavy Noble Gas Detectors for Long-Term Monitoring and Monitoring Air
PI: Dr. John D. Valentine *Institution:* Georgia Institute of Technology
Student Researchers: 4

Project: 64896

Title: Decontamination of Radionuclides from Concrete During and After Thermal Treatment
PI: Dr. Brian P. Spalding *Institution:* Oak Ridge National Laboratory
Student Researchers: 1

Project: 64912

Title: Improved Decontamination: Interfacial, Transport, and Chemical Properties of Aqueous Surfactant Cleaners
PI: Dr. David W. DePaoli *Institution:* Oak Ridge National Laboratory
Student Researchers: 3

Project: 64931

Title: Microbially Promoted Solubilization of Steel Corrosion Products and Fate of Associated Actinides
PI: Dr. Yuri A. Gorby *Institution:* Pacific Northwest National Laboratory
Student Researchers: 3

Project: 64946

Title: Mechanisms of Radionuclide-Hydroxycarboxylic Acid Interactions for Decontamination of Metallic Surfaces
PI: Dr. A.J. Francis *Institution:* Brookhaven National Laboratory
Student Researchers: 2

Project: 64947

Title: Contaminant-Organic Complexes, Their Structure and Energetics in Surface Decontamination Processes
PI: Dr. Calvin C. Ainsworth *Institution:* Pacific Northwest National Laboratory
Student Researchers: 2

Project: 64965

Title: Supercritical Carbon Dioxide-Soluble Ligands for Extracting Actinide Metal Ions from Porous Solids
PI: Dr. Mark D. Dietz *Institution:* Argonne National Laboratory
Student Researchers: 2

Project: 64979

Title: Decontamination and Decommissioning of PCB Sites at DOE: Extraction, Electrokinetics, and Hydrothermal Oxidation

PI: Dr. Edward A. Hamilton *Institution:* SCUREF

Student Researchers: 4

Project: 65001

Title: Development of Novel, Simple Multianalyte Sensors for Remote Environmental Analysis

PI: Dr. Sanford A. Asher *Institution:* University of Pittsburgh

Student Researchers: 3

Project: 65004

Title: Real-Time Identification and Characterization of Asbestos and Concrete Materials with Radioactive Contamination

PI: Dr. George Xu *Institution:* Rensselaer Polytechnic Institute

Student Researchers: 3

Project: 65328

Title: Electrically Driven Technologies for Radioactive Aerosol Abatement

PI: Dr. David W. DePaoli *Institution:* Oak Ridge National Laboratory

Student Researchers: 3

Project: 65339

Title: Ion Recognition Approach to Volume Reduction of Alkaline Tank Waste by Separation and Recycle of Sodium Hydroxide and Sodium Nitrate

PI: Dr. Bruce A. Moyer *Institution:* Oak Ridge National Laboratory

Student Researchers: 4

Project: 65340

Title: Detection and Characterization of Chemicals Present in Tank Waste

PI: Dr. P. G. Datskos *Institution:* Oak Ridge National Laboratory

Student Researchers: 4

Project: 65351

Title: Solution Effects on Cesium Complexation with Calixarene Crown Ethers from Liquid to Supercritical Fluids

PI: Dr. Chien M. Wai *Institution:* University of Idaho

Student Researchers: 3

Project: 65352

Title: Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation

PI: Dr. Sue B. Clark *Institution:* Washington State University

Student Researchers: 2

Project: 65366

Title: Physical, Chemical and Structural Evolution of Zeolite-Containing Waste Forms Produced From Metakaolinite and Calcined HLW

PI: Dr. Michael Grutzeck *Institution:* Pennsylvania State University

Student Researchers: 1

Project: 65410

Title: Rapid Migration of Radionuclides Leaked from High-Level Waste Tanks: A Study of Salinity Gradients, Wetted Path Geometry and Water Vapor Transport

PI: Dr. Anderson L. Ward *Institution:* Pacific Northwest National Laboratory

Student Researchers: 2

Project: 65411

Title: Precipitation and Deposition of Aluminum-Containing Phases in Tank Wastes

PI: Dr. Jun Liu *Institution:* Pacific Northwest National Laboratory

Student Researchers: 1

Project: 65421

Title: Correlation of Chemisorption and Electronic Effects for Metal/Oxide Interfaces: Transducing Principles for Temperature-Programmed Gas Microsensors

PI: Dr. Stephen Semancik *Institution:* National Institute of Standards & Technology -

Student Researchers: 4

Project: 65422

Title: Modeling of Spinel Settling in Waste Glass Melter

PI: Dr. Pavel Hrma *Institution:* Pacific Northwest National Laboratory

Student Researchers: 3

Project: 65425

Title: Mass Spectrometric Fingerprinting of Tank Waste Using Tunable, Ultrafast Infrared Lasers

PI: Dr. Richard F. Haglund *Institution:* Vanderbilt University

Student Researchers: 2

Project: 65435

Title: Millimeter-Wave Measurements of High Level and Low Activity Glass Melts

PI: Dr. Paul P. Woskov *Institution:* Massachusetts Institute of Technology

Student Researchers: 3

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Communications

EMSP COMMUNICATION PRODUCTS

One of the goals of the EMSP is to focus the nation's science infrastructure on critical Department of Energy environmental problems. One of the "tried and true" ways to increase the general body of knowledge within the scientific community is through publication of research methods, results, and issues. EMSP research has provided a basis for numerous information exchanges through this method. EMSP researchers and staff have developed 950 journal articles, papers, presentations, and other communication products. 133 articles have been submitted for review, and many additional news articles and press releases are either in development or planned as research within the program matures. The numbers of known publications and presentations as of December 31, 1999 are as follows:

- 329 Journal Articles
- 39 Other (Encyclopedias, manuscripts)
- 55 Papers
- 4 Patent disclosures and applications
- 17 Posters
- 368 Presentations
- 5 Press Releases
- 98 Proceeding Contributions
- 35 Reports

NOTE: In instances where an author was not identified for a particular communication product, the PI of the respective program has been listed as the author.

Project: 54506

Title: Acid-Base Behavior in Hydrothermal Processing of Wastes
PI: Dr. Keith P. Johnston *Institution:* University of Texas at Austin

Publication Type: Journal

Chlistunoff, J. B. & Johnston, K. P. (1999). UV-Vis spectroscopic determination of the dissociation constant of bichromate from 160°C to 400°C. Journal of Phys. Chem. B. 102, 3993-4003.

Chlistunoff, J. B., Ziegler, K. J., Lasdon, L., & Johnston, K. P. (1999). Nitric/ nitrous acid equilibria in supercritical water. Journal of Phys. Chem. B. 103, 1678-1688.

Johnston, K. P. & Chlistunoff, J. B. (1998). Neutralization of acids and bases in subcritical and supercritical water: Acetic acid and HCl. Journal of Supercritical Fluids, 12, 155-64.

Ziegler, K. J., Lasdon, L., Chlistunoff, J., & Johnston, K. P. (1999, in press). Optimization models for determining nitric acid equilibria in supercritical water. Computers and Chemistry.

Publication Type: Report

Johnston, K. P. & Rossky, P. J. (1999, in press). Solution chemistry in supercritical water: spectroscopy and simulation. In E. Kiran (Ed.), NATO Adv. Study Institute on Supercritical Fluids.

Project: 54546

Title: Engineered Antibodies for Monitoring of Polynuclear Aromatic Hydrocarbons
PI: Dr. Alexander E. Karu *Institution:* University of California at Berkeley

Publication Type: Journal

Guo, F., Li, Q. X., & Alcantara-Licudine, J. P. (1999). A simple Na4 EDTA-assisted sub/supercritical fluid extraction procedure for quantitative recovery of polar analytes in soil. Anal. Chem. 71, 1309-1315.

Li, K., Chen, R., Zhao, B., Liu, M., Karu, A. E., Roberts, V. A., & Li, Q. X. (1999). Monoclonal antibody-based enzyme-linked immunosorbent assays for part-per-billion determination of polycyclic aromatic hydrocarbons: Effects of haptens and formats on sensitivity and specificity. Anal. Chem. 71, 302-309.

Liu, M., Li, Q. X, & Rechnitz, G. A. (1999). Flow injection immunosensing of polycyclic aromatic hydrocarbon with a quartz crystal microbalance. Analyt. Chim. Acta. 387, 29-38.

Liu, M., Li, Q. X, & Rechnitz, G. A. (1999, in press). Gold electrode modification with thiolated hapten for the design of amperometric and piezoelectric immunosensors. Electrochem. Anal.

Liu, M., Rechnitz, G. A., Li, K. & Li, Q. X. (1998). Capacitive immunosensing of polycyclic aromatic hydrocarbon and protein conjugates. Anal. Lett. 31, 2025-2038.

Publication Type: Poster

Karu, A. E., Li, Q. X., & Roberts, V. (1998, July 27-30). Engineered antibodies for monitoring of polynuclear aromatic hydrocarbons. Poster presented at Department of Energy Environmental Science Management Program Workshop. Chicago, IL. http: //www.doe.gov/em52/1998posters/id54546.pdf.

Publication Type: Presentation

Li, Q. X., Li, K., Thomas, S. & Li, H. (1999, Aug. 22-26). Application of immunochemical methods for the analysis of polynuclear aromatic hydrocarbons in the environment (Abstract No. NUCL0047). Symposium on First Accomplishments of the Environmental Management Science Program, 218th National Meeting of the American Chemical Society. New Orleans, LA.

Pellequer, J.-L., Zhao, B., Kao, H.-I., Karu, A. E., & Roberts, V. A. (1999, Aug. 22-26). Cation-pi interactions in antibody binding of polynuclear aromatic hydrocarbons (Abstract No. 36750). Symposium on First Accomplishments of the Enviironmental Management Science Program, ACS Div. of Nuclear Chemistry and Technology, 218th National Meeting of the American Chemical Society. New Orleans, LA.

Project: 54571

Title: Removal of Heavy Metals and Organic Contaminants from Aqueous Streams by Novel Filtration Methods

PI: Dr. Nelly M. Rodriguez *Institution:* Northeastern University

Publication Type: Journal

Anderson, P. E. & Rodriguez, N. M. (1999, in press). Growth of graphie nanofibers from the decomposition of CO/H2 over silica supported iron-nickel particles. J. Materials Research.

Project: 54576

Title: On the Inclusion of the Interfacial Area Between Phases in the Physical and Mathematical Description of Subsurface Multiphase Flow

PI: Dr. William G. Gray *Institution:* University of Notre Dame

Publication Type: Journal

Gray, W. G. (1999, in press). Macroscale equilibrium conditions for two-phase flow in porous media. International Journal of Multiphase Flow.

Publication Type: Other

Soll, W. E., Gray, W. G. & Tompson, A. F. B. (1998). Influence of wettability on constitutive relations and its role in upscaling. In V. N. Burganos, et. al. (Eds.), Computational Methods in Water Resources XII, Computational Mechanics Publications, Southampton, Vol. 1, 413-420

Publication Type: Paper

Gray, W. G. (1999, Jan.). Thermodynamics and constitutive theory for multiphase porous-media flow considering internal geometric constraints. Advances in Water Resources, 22(5), 521-547.

Gray, W. G., & Hassanizadeh, S. M. (1998, July). Macroscale continuum mechanics for multiphase porous-media flow including phases, interfaces, common lines, and common points. Advances in Water Resources, 21(4), 261-281.

Muccino, J. C., Gray, W. G., & Ferrand, L. A. (1998, Aug.). Toward an improved understanding of multiphase flow in porous media. Reviews of Geophysics, 36(3), 401-422.

Project: 54585

Title: Permanganate Treatment of DNAPLs in Reactive Barriers and Source Zone Flooding Schemes

PI: Dr. Frank W. Schwartz *Institution:* Ohio State University

Publication Type: Journal

Yan, Y. E. & Schwartz, F. W. (1999). Oxidative degradation and kinetics of chlorinated ethylenes by potassium permanganate. Journal of Contaminant Hydrology. 37(3-4), 343-365.

Publication Type: Paper

Seol, Y. & Schwartz, F. W. (1999, Oct. 25-28). Phase transfer catalyst enhanced permanganate oxidation of trichloroethylene. Abstract for Annual conference of the Geological Society of America. Denver, CO.

Project: 54621

Title: Chemical Speciation of Strontium, Americium, and Curium in High Level Waste: Predictive Modeling of Phase Partitioning During Tank Processing

PI: Dr. Andrew R. Felmy *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Felmy, A. R. & Mason, M. J. (1998). The displacement of strontium from organic chelates by hydroxide, carbonate, and calcium in concentrated electrolytes. Journal of Solution Chemistry, 27(5), 435-454.

Felmy, A. R. & Rai, D. (1999, in press). Application of Pitzer's equations for modeling the aqueous thermodynamics of actinide species: A review. Invited paper for the special memorial edition of the Journal of Solution Chemistry in honor of Professor Kenneth Pitzer.

Felmy, A. R., Dixon, D. A., Rustad, J. R., Mason, M. J. & Onishi, L. M. (1998). The hydrolysis and carbonate complexation of strontium and calcium in aqueous electrolytes: Use of molecular modeling calculations in the development of aqueous thermodynamic models. Journal of Chemical Thermodynamics 30, 1103-1120.

Oakes, C. S., Sterner, S. M. & Felmy, A. R. (1999, in press). Thermodynamic properties of aqueous calcium nitrate [Ca(NO3)2] to 373K including new enthalpy of dilution data. Journal of Chemical Thermodynamics.

Sterner, S. M., Felmy, A. R., Oakes, C. S., & Pitzer, K. S. (1998). Correlation of thermodynamic data for aqueous electrolyte solutions to very high ionic strength using INSIGHT: Vapor saturated water activity in the system CaCl2-H2O to 250 ° C and solid saturation. International Journal of Thermophysics, 193, 761-770.

Publication Type: Presentation

Felmy, A. R., Choppin, G. R., Dixon, D. A., & Campbell, J. A. (1998, Jul. 27-30). Chemical speciation of strontium, americium, and curium in high-level waste: Predictive modeling of phase partitioning during tank processing. Two presentations and one poster. Presentations to the Hanford Tanks Site Technology Coordination Group (STCG) on November 10, 1998, and to PNNL staff on January 21, 1998. Poster presentation at the EMSP Principal Investigators Workshop, Chicago, IL.

Felmy, A. R. & Mason, M. J. (1998, Aug. 9-14). The aqueous complexation of Eu(III) with organic chelating agents at high base and high ionic strengths: Metal-chelate displacement induced by hydrolysis and precipitation reactions. 53rd Calorimetry Conference. Midland, MI.

Felmy, A. R., Dixon, D. A. & Mason, M. J. (1997, Aug. 3-8). The complexation of alkaline earth cations by organic chelates at high ionic strength: Competitive effects of hydrolysis and carbonate complextion. 52nd Calorimetry Conference. Asilomar, CA.

Felmy, A. R., Dixon, D. A. & Mason, M. J. (1999, Mar. 21-25). Aqueous complexation of Eu(III) with organic chelating agents at high base concentration: Molecular and thermodynamic modeling results. 217th ACS National Meeting. Anaheim CA.

Felmy, A. R., Dixon, D. A., Campbell, J. A. & Mason, M. J. (1997, Sept. 7-11). The effects of OH, CO3, and Ca on the displacement of strontium from organic chelates: Implications for waste processing. 214th ACS National Meeting. Las Vegas, NV.

Felmy, A. R., Dixon, D. A., Rustad, J. R., Mason, M. J. & Onishi, L. M. (1997, Aug. 3-8). The use of molecular modeling calculations to improve the development of thermodynamic models: Hydrolysis, carbonate, and EDTA complexation of alkaline earth cations. 52nd Calorimetry Conference. Asilomar, CA.

Oakes, C. S. & Felmy, A. R. (1997, Aug. 3-8). Thermodynamics of [Na4EDTA+NaOH]{aq}, including new isopiestic measurements, to 373K, 0.1MPa, and stoichiometric ionic strengths of 18 . 9mol . kg -1. 52nd Calorimetry Conference, Asilomar, CA.

Oakes, C. S. & Felmy, A. R. (1998, Aug. 9-14). Thermodynamics of [Na4EDTA+NaOH]{aq}, including new isopiestic and enthalpy of dilution measurements. 53rd Calorimetry Conference. Midland, MI.

Petersen, C. E., Campbell, J. A., Felmy, A. R., Wahl, K. L. & Finch, J. W. (1998, May 31-June 4). Analysis of metal-organic complexes using CE/MS. 46th American Society of Mass Spectrometry Meeting. Orlando, FL.

Sterner, S. M., Felmy, A. R. & Pitzer, K. S. (1997, Jun. 22-27). Correlation of thermodynamic data for aqueous electrolyte solutions to very high ionic strength using INSIGHT: Vapor saturated water activity in the system CaCl2-H2O to 250 ° C and solid saturation. Thirteenth Symposium on Thermophysical Properties. Boulder, CO.

Sterner, S. M., Felmy, A. R., Oakes, C. S., Simonson, J. M., & Pitzer, K. (1997, Aug. 3-8). Thermodynamics of aqueous CaCl2 to 250 ° C, 400 bars and solid saturation. 52nd Calorimetry Conference. Asilomar, CA.

Project: 54628

Title: Colloidal Agglomerates in Tank Sludge: Impact on Waste Processing
PI: Dr. Joel M. Tingey *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Tingey, J. M., Bredt, P. R., & Shekarriz, R. (1999, Mar.). Rheology and settling behavior of Hanford tank wastes and the resulting process streams. Rheology in Mineral Industry II. Kahuku, Oahu, HI.

Tingey, J. M., Bunker, B. C., Graff, G. L., Keefer, K. D., Lea, A. S., & Rector, D. R. (1998, Nov.). Colloidal agglomerates in tank sludge and their impact on waste processing. Materials Research Society Fall Meeting. Boston, MA.

Tingey, J. M., Graff, G. L., & Rector, D. R. (1999, Mar.). Effect of colloidal aggregation on sedimentation and rheology in highly basic, high ionic strength salt solutions. Rheology in Mineral Industry II. Kahuku, Oahu, HI.

Project: 54635

Title: Molecular-Level Process Governing the Interaction of Contaminants with Iron and Manganese Oxides
PI: Dr. Scott A. Chambers *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Brown, G. E. Jr., et. al. (1999). Metal oxide surfaces and their interactions with aqueous solutions and microbial organisms. Chem. Rev. 99, 77-174.

Chambers, S. A. & Liang, Y. (1999). Growth of • -MnO2 films on TiO2(110) by oxygen-plasma-assisted molecular beam epitaxy. Surf. Sci. Spect. 420, 123.

Chambers, S. A., & Joyce, S. A. (1999). Surface termination, composition, and reconstruction of Fe3O4(001) and • -Fe2O3(001). Surf. Sci. Spect. 420, 111.

Chambers, S. A., Gao, Y. & Kim, Y. J. (1998). Fe 2p core-level spectra for pure, epitaxial • -Fe2O3(0001), • -Fe2O3(001), and Fe3O4(001). Surf. Sci. Spect. 5, 219.

Foster, N. S., Amonette, J. E., & Autrey, S. T. (1999, in press). In-situ detection of chromate using photoacoustic spectroscopy. Appl. Spectrosc.

Foster, N. S., Amonette, J. E., & Autrey, S. T. (1999, in press). In-situ detection of chromate using photoacoustic spectroscopy. Appl. Spectrosc.

Foster, N. S., Autrey, S. T., Amonette, J. E., Small, J. R., & Small, E. W. (1999). Laser photoacoustic spectroscopy: A versatile absorption spectroscopic technique. Am. Lab. 31, 96s-108s.

Grolimund, D., et. al. (1999, in press). Identification of Cr species at the aqueous solution hematite interface after Cr(VI)-Cr(III) reduction using GI-XAFS and Cr L-edge NEXAFS. Journal of Synchrotron Radiation.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1999). Reaction of water with the (100) and (111) surfaces of Fe3O4." Surface Science.

Kendelewicz, T., Liu, P., Doyle, C. S., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1999). "X-ray absorption and photoemission study of the adsorption of aqueous Cr(VI) on single crystal hematite and magnetite surfaces." Surf. Sci. Spect. 424, 219.

Liu, P., Kendelewicz, T., Brown, G. E. Jr., Nelson, E. J. & Chambers, S. A. (1998). Reaction of water vapor with • -Al2O3(0001) and • -Fe2O3(0001) surfaces: Synchrotron x-ray photoemission studies and thermodynamic calculations." Surf. Sci. Spect. 417, 53.

Rustad, J. R., Dixon, D. A., Kubicki, J. D., & Felmy, A. R. (1999, in press). Gas-phase acidities of tetrahedral oxyacids from ab initio electronic structure calculations. J. Phys. Chem.

Rustad, J. R., Wasserman, E., & Felmy, A. R. (1999, in press). A molecular dynamics investigation of surface reconstruction on magnetite (001)." Surf. Sci. Spect.

Thevuthasan, S., et. al. (1999). Surface structure of MBE-grown • -Fe2O3(0001) by intermediate-energy x-ray photoelectron diffraction. Surf. Sci. Spect. 425, 276-286.

Yi, S. I., Liang, Y. & Chambers, S. A. (1999). Effect of growth rate on the nucleation of • -Fe2O3 on • -Al2O3(0001) by oxygen-plasma-assisted molecular beam epitaxy. J. Vac. Sci. Technol. A.

Publication Type: Presentation

Amonette, J. E., Foster, N. S., William, B. K., & Taylor, A. E. (1999, Mar. 21-25). Trace-level chromate sorption dynamics at hematite surfaces: A spectroscopic approach. 217th National Meeting of the American Chemical Society. Anaheim, CA.

Amonette, J. E., Foster, N. S., William, B. K., & Taylor, A. E. (1999, Jun.). Competitive trace-level sorption of chromate and phosphate to hematite surfaces: A spectroscopic approach. 36th Annual Meeting of the Clay Minerals Society. Purdue University. West Lafayette, IN.

Brown, G. E. Jr., et. al. (1999, Mar.). Characterization of adsorbed chemical species at mineral surfaces. 217th American Chemical Society Meeting. Anaheim, CA.

Chambers, S. A. (1998, Oct.). Molecular beam epitaxial growth and surface structure determination of Fe and Mn oxides. Invited presentation at the Center for Catalysis and Surface Structure. Northwestern University. Evanston, IL.

Chambers, S. A., Thevuthasan, S., Kim, Y. J., Joyce, S. A., & Liang, Y. (1998, Aug.). Surface structure determination of MBE grown iron and manganese oxides. Invited presentation at the National Meeting of the American Chemical Society. Boston, MA.

Chambers, S. A.,Thevuthasan, S., & Joyce, S. A. (1999, Jan.). Structure and reactivity of MBE-grown Fe oxides. Invited presentation at the First International Conference on Oxide Surfaces. Elmau, Germany.

Grolimund, D., et. al. (1998, Jul.). Identification of Cr species at the solution-hematite interface after Cr(VI)-Cr(III) reduction using GI-XAFS and Cr L-edge NEXAFS. 10th International XAFS Conference. Chicago, IL.

Grolimund, D., Fitts, J. P., Trainor, T. P., Brown, G. E. Jr., & Chambers, S. A. (1999, Mar.). Identification of Cr species at the aqueous solution-oxide interface using grazing-incidence XAFS. 217th American Chemical Society Meeting. Anaheim, CA.

Joyce, S. A., Thevuthasan, S., & Chambers, S. A. (1999, Mar. 21-25). Growth and structure of synthetic iron oxide mineral surfaces. 217th National Meeting of the American Chemical Society. Anaheim, CA.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., & Nelson, E. J. (1998, Aug.). Reaction of water with (100) and (111) surfaces of magnetite (Fe3O4). International Conference on Surface Science 10. Birmingham, United Kingdom.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Chambers, S. A., & McCarthy, M. I. (1998, Aug.). “Hydroxylation of the surfaces of simple metal oxides: Spectroscopic and thermodynamic analysis. Goldschmidt Conference. Toulouse, France.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1998, Aug.). Reaction of water with clean (0001) and (1-102) surfaces of • -Fe2O3. International Conference on Surface Science 10. Birmingham, United Kingdom.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1998, Aug.). Fe L2,3 and O K near edge structure of iron oxides and hydroxides. International Conference on Surface Science 10. Birmingham, United Kingdom.

Kendelewicz, T., Liu, P., Brown, G. E. Jr., Nelson, E. J., & Chambers, S. A. (1998, Aug.). Reduction of the (0001) surface of hematite (• -Fe2O3) prepared under UHV conditions. International Conference on Surface Science 10. Birmingham, United Kingdom.

McCready, D. E., (1998, Jun.). Rutherford backscattering and channeling studies of epitaxially grown iron oxide films on various substrates. Surface Analysis/8th Annual Pacific Northwest Symposium.

Rustad, J. R. (1999, Aug.). Molecular simulation of the iron oxide-water interface. Invited presentation at the American Chemical Society Meeting. New Orleans, LA.

Rustad, J. R., Wasserman, E., & Joyce, S. A. (1999, Mar. 21-25). Structure and energetics of the magnetite(001) surface insights from molecular dynamics calculations. 217th National Meeting of the American Chemical Society. Anaheim, CA.

Thevuthasan S. (1998, Nov.). Rutherford backscattering and channeling studies of Al and Mg diffusion in iron oxide thin films. Invited presentation at the Fifteenth International Conference on the Application of Accelerators. Denton, TX.

Thevuthasan, S., et. al. (1998, Jun.). The surface structure determination of • -Fe2O3 by intermediate-energy x-ray photoelectron diffraction. Surface Analysis/ 8th Annual Pacific Northwest Symposium.

Thevuthasan, S., et. al. (1998, Nov.). The surface structure determination of • -Fe2O3 (0001) by low-energy x-ray photoelectron diffraction. 45th National Symposium of the American Vacuum Society.

Thevuthasan, S., Jiang, W., McCready, D. E., & Chambers, S. A. (1998, Nov.). Rutherford backscattering and channeling studies of Al and Mg diffusion in iron oxide thin films. 45th National Symposium of the American Vacuum Society.

Thevuthasan, S., McCready, D. E., Jiang, W., Yi, S. I., & Chambers, S. A. (1999, Jul.). Ion beam analysis of interface reactions in iron oxide thin films. Invited presentation at the Fourteenth International Conference on Ion Beam Analysis (IBA-14). Dresden, Germany.

Publication Type: Proceeding

Chambers, S. A., & Liang, Y. (1998, Nov.). Growth of • -MnO2 films on TiO2(110) by oxygen-plasma- assisted molecular beam epitaxy.” 45th International Symposium of the American Vacuum Society. Baltimore, MD.

Project: 54639

Title: Development of an In-Situ Microsensor for the Measurements of Chromium and Uranium in Groundwater at DOE Sites

PI: Dr. Joseph Wang *Institution:* New Mexico State University

Publication Type: Journal

Wang, J., Bhada, R., Lu, J., & MacDonald, D. (1998). Remote sensor for monitoring TNT in natural waters. Anal. Chim. Acta, 361, 85.

Wang, J., Lu, J., & Augelli, M. (1999). In-situ flow probe for improving the performance of electrochemical stripping analysis. Fres. J. Anal. Chem., 364, 28.

Wang, J., Lu, J., Tian, B., MacDonald, D., & Olsen, K. (1999). Flow probe for in-situ electrochemical monitoring of trace chromium. Analyst, 124, 349.

Wang, J., Tian, B., & Lu, J. (1998). Electrochemical flow sensor for in-situ monitoring of total metal concentration. Anal. Communications, 35, 241.

Wang, J., Tian, B., Lu, J., & MacDonald, D. (1998). Remote electrochemical sensor for monitoring trace mercury. Electroanalysis 10, 399.

Wang, J., Tian, B., Lu, J., Yarnitsky, C., Olsen, K., & Bennet, W. (1999). Stripping analysis into the 21st century: Faster, smaller, simpler, and better. Anal. Chim. Acta, 385, 429.

Project: 54646

Title: Interfacial Radiolysis Effects in Tank Waste Speciation

PI: Dr. Thomas M. Orlando *Institution:* Pacific Northwest National Laboratory

Publication Type: Paper

Orlando, T. M. (1999, March 21-26). Reaction of NO_2 with organic complexants in alkaline solutions. 217th American Chemical Society National Meeting, Anaheim, CA.

Project: 54656

Title: Mixing Processes in High-Level Waste Tanks

PI: Dr. Per F. Peterson *Institution:* University of California at Berkeley

Publication Type: Presentation

Christensen, J. & Peterson, P. F. (1999, Oct. 3-8). A one-dimensional lagrangian model for large-volume mixing. Accepted for the Ninth International Topical Meeting on Nuclear Reactor Thermal Hydraulics. San Francisco, CA.

Kuhn, S. Z., Lee, C., & Peterson, P. F. (1999, Oct. 3-8). “Stratification from buoyancy-driven exchange flow through horizontal partitions in a liquid tank. Accepted for the Ninth International Topical Meeting on Nuclear Reactor Thermal Hydraulics. San Francisco, CA.

Publication Type: Proceeding

Peterson, P. F. & Gamble, R. E. (1998). Scaling for forced-convection augmentation of heat and mass transfer in large enclosures by injected jets. Transactions of American Nuclear Society, 78, 265-266.

Project: 54666

Title: Mechanisms, Chemistry, and Kinetics of Anaerobic Biodegradation of cDCE and Vinyl Chloride

PI: Dr. Perry L. McCarty *Institution:* Stanford University

Publication Type: Journal

Haston, Z. C. & McCarty, P. L. (1999). Chlorinated ethene half-velocity coefficients (K S) for reductive dehalogenation. Environmental Science and Technology, 33(2), 223-226.

Rosner, B., McCarty, P. L., & Spormann, A. M. (1997). In vitro studies on reductive vinyl chloride dehalogenation by an anaerobic mixed culture. Appl. Environ. Microbiol., 63 (11): 4139-4144.

Yang, Y. & McCarty, P. L. (1998). Competition for hydrogen within a chlorinated solvent dehalogenating mixed culture. Environmental Science and Technology, 32(22), 3591-3597.

Yang, Y. & McCarty, P. L. (1999, in press). Response to "Comment on competition for hydrogen within a chlorinated solvent dehalogenating anaerobic mixed culture." Environmental Science & Technology.

Project: 54672

Title: Radiation Effects in Nuclear Waste Materials

PI: Dr. William J. Weber *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Gorretta, K. C., et. al. (1999). Solid-particle erosion of Portland cement and concrete. Wear 224, 106-112.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1998). X-ray absorption fine structure of aged, Pu-doped glass and ceramic waste forms. Journal of Nuclear Materials, 254: 175-184.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1998). U and Pu LIII XAFS of Pu-doped glass and ceramic waste forms. Journal of Alloys and Compounds, 271-273, 240-243.

Weber, W. J., Ewing, R. C., & Meldrum, A. (1997). The kinetics of alpha-decay-induced amorphization in zircon and apatite containing weapons-grade plutonium or other actinides. Journal of Nuclear Materials, 250, 147-155.

Williford, R. E., Devanathan, R., & Weber, W. J. (1998). Computer simulation of displacement threshold energies for several ceramic materials. Nuclear Instruments and Methods B 141, 98-103.

Williford, R. E., Weber, W. J., Devanathan, R., & Cormack, A. N. (1999, in press). Native vacancy migrations in zircon. Journal of Nuclear Materials.

Publication Type: Other

Begg, B. D., et. al. (1999, in press). Heavy-ion irradiation effects in pyrochlores. In Smith, G. L., Chandler, G. T., & Mobasher, B. (Eds.), Waste Management Science and Technology in the Ceramic and Nuclear Industries. The American Ceramic Society. Westerville, OH.

Chen, X. & Birtcher, R. C. (1999, in press). Bubble formation and growth in nuclear waste glasses. In Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.). Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540. Warrendale, PA.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jónsson, H. (1999, in press). Vacancy migration and excitons in silica polymorphs. In Smith, G. L., Chandler, G. T., & Mobasher, B. (Eds.). Mater. Waste Management Science and Technology in the Ceramic and Nuclear Industries. The American Ceramic Society. Westerville, OH.

Publication Type: Paper

Williford, R. E. & Weber, W. J. (1999, Apr. 25-28). Defect formation and migration energetics in disordered Gd2Ti2O7. The 101st Meeting of The American Ceramic Society. Indianapolis, IN.

Publication Type: Presentation

Begg, B. D., et. al. (1999, Apr. 25-28). Heavy-ion irradiation effects in pyrochlores. The 101st Meeting of The American Ceramic Society. Indianapolis, IN.

Begg, B. D., Hess, N. J., & Weber, W. J. (1999, Apr. 22-23). XAS and XRD characterization of annealed Pu-doped zircon. CEA Meeting on HLW and Pu Immobilization. Saclay, France.

Chen, X., Birtcher, R. C., & Donnelly, S. E. (1998, Nov. 30 - Dec. 4). Bubble formation and growth in nuclear waste glasses. Materials Research Society Annual Meeting. Boston, MA.

Corrales, L. R. & Song, J. (1997, Sept.). Molecular dynamics simulations of excitons in glasses. CEA/VALHRO Summer School. Mejannes le Clap, France.

Corrales, L. R. (1997, Oct.). Lattice theories and molecular dynamics simulations of glasses. Department of Chemistry, University of Maryland. College Park, MD.

Corrales, L. R. (1997, Oct.). Molecular dynamics simulations of defects and excitons in glasses. American Ceramics Society, Glass and Optical Materials Division Meeting. Williamsburg, VA.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jónsson, H. (1999, Apr. 25-28). The formation and migration energetics of radical defects in silica polymorphs. Invited presentation at the 101st Meeting of The American Ceramic Society. Indianapolis, IN.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jónsson, H. (1999, Mar. 21-25). Migration of oxygen vacancy radical defects and self-trapped excitons in silica. Invited presentation at the 217th American Chemical Society Meeting. Anaheim, CA.

Corrales, L. R., VanGinhoven, R. M., Song, J., & Jónsson, H. (1998, Nov. 30 - Dec. 4). Vacancy migration barrier energetics and pathways in silica. Materials Research Society Annual Meeting. Boston, MA.

Devanathan, R., Weber, W. J., & Boatner, L. A. (1997, Dec. 1-5). Response of zircon to electron and Ne + irradiation. Materials Research Society Annual Meeting. Boston, MA.

Devanathan, R., Weber, W. J., & Williford, R. E. (1998, Nov. 30 - Dec. 4). Amorphization of Gd2Ti2O7 by energetic heavy ion irradiation. Materials Research Society Annual Meeting. Boston, MA.

Fortner, J. A., Hanchar, J. M., Badyal, Y., Price, D. L., & Weber, W. J. (1998, Nov. 30 - Dec. 4). Structural analysis of a completely amorphous 238 Pu-doped zircon by neutron diffraction. Materials Research Society Annual Meeting. Boston, MA.

Hess, N. J., Maupin, G. D., & Weber, W. J. (1998, Nov. 30 - Dec. 4). Spectroscopic studies of gamma-irradiated glass waste forms. Materials Research Society Annual Meeting, Boston, MA.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1997, Sept. 21-26). U and Pu LIII XAFS of Pu-doped glass and ceramic waste forms. International Conference on Actinides ‘97. Baden-Baden, Germany.

Song, J. & Corrales L. R. (1998, Mar. 16-20). Simulation of exciton processes in networked materials. March APS National Meeting. Anaheim, CA.

Song, J., Corrales, L. R., & Jónsson, H. (1998, Nov. 30 - Dec. 4). Exploring the excited states of vacancy defects in silica. Materials Research Society Annual Meetin. Boston, MA.

Thevuthasan, S., Jiang, W., McCready, D. E., & Weber, W. J. (1998, Nov. 30 - Dec. 4). Damage accumulation and thermal recovery in SrTiO3 implanted with various ions. Materials Research Society Annual Meeting. Boston, MA.

Weber, W. J. & Corrales, L. R. (1998, July 27-30). Radiation effects in nuclear waste forms. DOE Environmental Management Science Program Scientific Workshop. Rosemont, IL.

Weber, W. J. & Devanathan, R. (1998, May 4-6). Effects of alpha decay on crystalline ceramic waste forms. American Ceramic Society Meeting. Cincinnati, OH.

Weber, W. J. (1988, July 27-30). EMSP projects in materials science. DOE Environmental Management Science Program Scientific Workshop. Rosemont, IL.

Weber, W. J. (1997, Dec. 1). Radiation effects in glass and ceramic waste forms. Invited presentation at the Massachusetts Institute of Technology. Cambridge, MA.

Weber, W. J. (1997, Dec. 11). Radiation effects in glass waste forms. Invited presentation at Argonne National Laboratory. Argonne, IL.

Weber, W. J. (1997, Feb. 20). Radiation effects from the incorporation of plutonium in glasses and ceramics. Invited presentation at Los Alamos National Laboratory. Los Alamos, NM.

Weber, W. J. (1998, Apr. 19-22). Effects of radiation on solid nuclear waste forms. Invited plenary lecture at the DOE Workshop on Research Needs and Opportunities in Radiation Chemistry. Chesterton, IN.

Weber, W. J. (1998, Apr. 3-4). Radiation effects from alpha decay in nuclear waste ceramics. Invited plenary lecture at the American Nuclear Society Northern Student Conference. Ann Arbor, MI.

Weber, W. J. (1998, Jan. 8). Radiation effects in crystalline waste form phases. Invited presentation at the Idaho National Engineering and Environmental Laboratory. Idaho Falls, ID.

Weber, W. J., et. al. (1998, Nov. 30 - Dec. 4). The effect of temperature and recoil spectra on amorphization in zircon. Materials Research Society Annual Meeting. Boston, MA.

Weber, W. J., Ewing, R. C., & Meldrum, A. (1998, Mar. 30 - Apr. 3). Radiation effects in nuclear waste ceramics. American Chemical Society Annual Meeting. Dallas, TX.

Weber, W. J., Hess, N. J., Conradson, S. D., & Vienna, J. D. (1997, Aug. 25-27). Self-radiation effects in glass and ceramic waste forms for the stabilization and disposition of plutonium. Topical Conference on Plutonium Futures - The Science. Santa Fe, NM.

Williford, R. E., Devanathan, R. & Weber, W. J. (1997, Sept. 14-19). Computer simulation of displacement threshold energies for several ceramic materials. 9th International Conference on Radiation Effects in Insulators. Knoxville, TN.

Williford, R. E., Weber, W. J., Devanathan, R., & Gale, J. D. (1998, Nov. 30 - Dec. 4). Oxygen vacancy migration in Gd2(Ti,Zr)2O7 pyrochlores. Materials Research Society Annual Meeting. Boston, MA.

Publication Type: Proceeding

Begg, B. D., Hess, N. J., & Weber, W. J. (1999, in press). XAS and XRD characterization of annealed Pu-doped zircon. In Meis, C. & Carpena, J. (Eds.), Proceedings of the CEA Meeting on HLW and Pu Immobilization, CEA/Saclay.

Corrales, L. R. & Song, J. (1998). Semi-empirical methodology to simulate exciton processes in glasses. Proceeds of the CEA/VALRHO Summer School on Glass: Scientific Research for High Performance Containment. CEA/Valrhô, Bagnols-sur-Cèze, France, 218-227.

Corrales, L. R., VanGinhoven, R. M., Song, J., & Jónsson, H. (1999). Vacancy migration barrier energetics and pathways in silica. In Bulatov, V. V., Diaz de la Rubia, T., Phillips, R., Kaxiras, E., & Ghoniem, N. (Eds.) Multiscale Modeling of Materials. Mater. Res. Soc. Symp. Proc. 538, Warrendale, PA. 317-321.

Devanathan, R., Weber, W. J., & Boatner, L. A.. (1998). Response of zircon to electron and Ne + irradiation. In Ma, E., Bellon, P., Atzmon, M., & Trivedi, R. (Eds.) Phase Transformations and Systems Driven far from Equilibrium. Mater. Res. Soc. Symp. Proc. 481, Warrendale, PA. 419-424.

Fortner, J. A., Hanchar, J. M., Badyal, Y., Price, D. L., & Weber, W. J. (1999, in press). Structural analysis of a completely amorphous 238 Pu-doped zircon by neutron diffraction. In Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.). Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Heinisch, H. L., Williford, R. E. & Weber, W. J. (1998, Nov. 30 - Dec. 4). Computer simulations of irradiation-induced defect accumulation and amorphization in zircon. Materials Research Society Annual Meeting. Boston, MA.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1998). X-ray absorption fine structure of aged, Pu-doped glass and ceramic waste forms. In McKinley, I. G. & McCombie, C. (Eds.), Scientific Basis for Nuclear Waste Management XXI. Mater. Res. Soc. Symp. Proc. 506, Warrendale, PA. 169-176.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1997, Sept. 28 - Oct. 3). X-ray absorption fine structure of aged, Pu-doped glass and ceramic waste forms. MRS Symposium, Scientific Basis for Nuclear Waste Management XXI. Davos, Switzerland.

Thevuthasan, S., Jiang, W., McCready, D. E., & Weber, W. J. (1999, in press). Damage accumulation and thermal recovery in SrTiO3 implanted with various ions. In Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Weber, W. J., et. al. (1999, in press). The effect of temperature and recoil spectra on amorphization in zircon. In Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Publication Type: Report

Weber, W. J., Hess, N. J., Conradson, S. D., & Vienna, J. D. (1997). Self-radiation effects in glass and ceramic waste forms for the stabilization and disposition of plutonium. Plutonium Futures - The Science. LA-13338-C, Los Alamos National Laboratory. Los Alamos, NM. 25-26.

Weber, W. J. & Corrales, L. R. (1997). Radiation effects in nuclear waste materials. Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. PNNL-11589, Pacific Northwest National Laboratory. Richland, WA. 43-52.

Weber, W. J. & Corrales, L. R. (1998). Radiation effects in nuclear waste materials. Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. PNNL-11889, Pacific Northwest National Laboratory. Richland, WA. 1.107-1.126.

Project: 54679

Title: Architectural Design Criteria for F-Block Metal Ion Sequestering Agents
PI: Dr. Benjamin P. Hay *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Clement, O., Rapko, B. M., & Hay, B. P. (1998). Structural aspects of metal-amide complexes. Coordination Chemistry Reviews 170, 203.

Falana, O. M., Koch, H. R., Roundhill, D. M., Lumetta, G. J., & Hay, B. P. (1998). Synthesis and extraction studies of 1,2- and 1,3-disubstituted butylcalix[4]Arene amides with oxyions: Geometric and conformational effects. Journal of the Chemical Society, Chemical Communications 503.

Hay, B. P., Clement, O., Sandrone, G., & Dixon, D. A. (1998). A MM3(96) force field for metal amide complexes. Inorganic Chemistry, 37, 5887.

Lumetta, G. L., McNamara, B. K., & Rapko, B. M. (1999, in press). Complexation of uranyl ion by tetrahexyl-malonamides: An equilibrium modeling and infrared spectroscopic study. Inorganica Chimica Acta.

McNamara, B. K., Lumetta, G. J. & Rapko, B. M. (1999, in press). Extraction of europium(III) ion with tetrahexylmalonamides. Solvent Extraction and Ion Exchange.

Rao, L., Xia, Y., Rapko, B. M., & Martin, P. F. (1998). Synergistic extraction of Eu(III) and Am(III) by thenoyltrifluoroacetone and neutral donor extractants: Octyl(phenyl)-N,N-diisobutylcarbonyl-methylphosphine oxide and 2,6-bis(diphenylphosphino)methyl pyridine N,P,P trioxide. Solvent Extraction and Ion Exchange, 16, 913.

Rapko, B. M., McNamara, B. K., Lumetta, G. J., Rogers, R. D., & Hay, B. P. (1999, in press). Coordination chemistry of lanthanide nitrates with N,N,N,N-tetramethylsuccinamide. Inorganic Chemistry.

Sandrone, G., Dixon, D. A., & Hay, B. P. (1999). C(sp 2)-C(sp 3) rotational barriers in simple amides: H2N-C(=O)-R, R = methyl, ethyl, i-propyl, t-butyl. Journal of Physical Chemistry, A 103, 893.

Sandrone, G., Dixon, D. A., & Hay, B. P. (1999). Conformational analysis of malonamide, N,N'-dimethylmalonamide, and N,N,N',N'-tetramethylmalonamide. Journal of Physical Chemistry, A.18: 3554

Wolf, N. J., et. al. (1999, in press). Synthesis of lower rim amine and carbamoyl substituted calixarenes as transfer agents for oxyions between an aqueous and a chloroform phase. Polyhedron.

Yordanov, A. & Roundhill, D. M. (1998). Solution extraction of transition and post-heavy and precious metals by chelate and macrocyclic ligands. Coordination Chemistry Reviews, 170, 93.

Yordanov, A. T., et. al. (1999). Derivatized calix[4]arenes as selective phase transfer extractants for heavy metal and oxyion salts. Comments on Inorganic Chemistry, 20, 163.

Publication Type: Other

Hay, B. P. & Clement, O. (1998). Metal complexes. Invited Book Chapter In Schleyer, P. R., et. al. (Eds.) The Encyclopedia of Computational Chemistry. John Wiley and Sons, Chichester, NY.

Publication Type: Presentation

Clement, O., Hay, B. P. Dixon, D. A., & Sandrone, G. (1998, Jun.). A MM3(96) force field for metal-amide complexes. West Coast Theoretical Chemistry Conference. Richland, WA.

Clement, O., Sandrone, G., Dixon, D. A., & Hay, B. P. (1998, Mar.). A MM3(96) force field for metal-amide complexes. 215th American Chemical Society National Meeting, Dallas, TX.

Clement, O., Sandrone, G., Dixon, D. A., & Hay, B. P. (1998, Jun.). A MM3(96) force field for metal-amide complexes. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Hay, B. P. (1998, Aug.). A points-on-a-sphere approach to model metal-ligand interactions with an extended MM3 model. Invited presentation at the 216th American Chemical Society National Meeting, Boston, MA.

Hay, B. P. (1998, Jul.) Architectural design criteria for f-block metal sequestering agents. Environmental Management Science Program Workshop. Chicago, IL.

Hay, B. P. (1998, Oct.). Ligand design with molecular mechanics. INEEL Science Integrated Workshop, Environmental Management Science Program. Idaho Falls, ID.

Hay, B. P. (1999, Jun.) The application of molecular mechanics in the design of metal ion sequestering agents. Invited presentation at the Metal Separation Technologies Beyond 2000: Integrating Novel Chemistry with Processing United Engineering Foundation Conference. Turtle Bay, Oahu, HI.

Hay, B. P., Dixon, D. A., & Sandrone, G. (1998, Jun.). A modified MM3(96) force field for simple amides and diamides. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Hay, B. P., Dixon, D. A., & Sandrone, G. (1998, Jun.). A modified MM3(96) force field for simple amides and diamides. West Coast Theoretical Chemistry Conference. Richland, WA.

Lumetta, G. J., McNamara, B. K., & Burgeson, E. (1997, Jun). Amide complexes of f-block elements. 21st Annual Actinide Separations Conference. Charleston, SC.

Lumetta, G. J., McNamara, B. K., & Rapko, B. M. (1998, Jun.). Binding of diamide ligands to f-block elements. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Lumetta, G. J., McNamara, B. K., & Rapko, B. M. (1998, Apr.). Binding of amide ligands to f-block elements. 22nd Annual Actinide Separations Conference. Chattanooga, TN.

Lumetta, G. J., McNamara, B. K., & Rapko, B. M. (1999, Mar.). Equilibrium modeling of the extraction of f-block elements by diamides. 217th American Chemical Society National Meeting. Anaheim, CA.

Rao, L., Zanonato, P., & Di Bernardo, P. (1998, Aug.). Thermodynamics of europium(III) complexation with alkyl-substituted diamides in organic solvents. 216th American Chemical Society National Meeting. Boston, MA.

Rapko, B. M. (1997, Apr.) Extraction of f-elements by phosphine oxide/pyridine N-oxide ligands. 213th American Chemical Society National Meeting. San Francisco, CA.

Rapko, B. M., et al. (1999, Mar.). Coordination chemistry of tetraalkyldiamides with f-block metal salts. 217th American Chemical Society National Meeting. Anaheim, CA.

Rapko, B. M., et. al. (1999, Jun.). Coordination chemistry of diamides with f-block metal salts. Metal Separation Technologies Beyond 2000: Integrating Novel Chemistry with Processing United Engineering Foundation Conference. Turtle Bay, Oahu, HI.

Rapko, B. M., Lumetta, G. J., McNamara, B. K., Rao, L., & Zanonato, P. L. (1997, Oct.). Determination of actinide and lanthanide binding constants with amides and diamides. Tenth Symposium on Separation Science and Technology for Energy Applications. Gatlinburg, TN.

Rapko, B. M., McNamara, B. K., Rogers, R. D., Lumetta, G. J., & Hay, B. P. (1998, Jun.). Coordination chemistry of lanthanide salts with N,N,N',N'-tetramethylsuccinamide and N,N,N',N'-tetrahexyl-succinamide. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Roundhill, D. M. (1998, May). New macrocycles for selective ion exchange. Metals Adsorption Workshop. Cincinnati, OH.

Roundhill, D. M. (1999, Mar.). Calixarene amines and amides as extractants for oxyions. 217th National American Chemical Society National Meeting. Anaheim, CA.

Yordanov, A. T., Wolf, N. J., Koch, H. F., & Roundhill, D. M. (1998, Jun.). Sulfur and nitrogen derivatized calix[4]arenes as selective phase transfer extractants for heavy metals and oxyions. Second Fargo Conference on Main Group Chemistry. Fargo, ND.

Zanonato, P. L. & Rao, L. (1997, Sept.). Complexation of Eu(III) by N,N,N',N'-tetra-alkyldiamides. 214th American Chemical Society National Meeting. Las Vegas, NV.

Publication Type: Proceeding

Hay, B. P. (1999, in press). The use of molecular mechanics in the design of metal ion sequestering agents. In Metal separation technologies beyond 2000: Integrating novel chemistry with processing. United Engineering Foundation. New York, NY.

Hay, B. P., Dixon, D. A., Lumetta, G. J., & Rapko, B. M. (1998). Environmental management science program workshop. CONF-980736, Environmental Management Science Program, U.S. Department of Energy, Office of Science and Risk Policy EM-52. Washington, D.C.

Rao, L., Xia, Y., Rapko, B. M., & Martin, P. L. (1997, Jun). Synergistic extraction of Eu(III) and Am(III) by TTA and the neutral donor extractants CMPO and NOPOPO. 21st Annual Actinide Separations Conference. Charleston, SC.

Publication Type: Report

Hay, B. P., Dixon, D. A., Lumetta, G. J., & Rapko, B. M. (1997). Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. Fiscal Year 1997 Mid-Year Progress Report. PNNL-11589, Pacific Northwest National Laboratory. Richland, WA.

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Lumetta, G. J., Rapko, B. M., & McNamara, B. K. (1999). The SX solver: A new computer program for analyzing solvent extraction equilibria. PNNL-12085, Pacific Northwest National Laboratory. Richland, WA.

Project: 54680

Title: The Migration and Entrapment of DNAPLs in Physically and Chemically Heterogeneous Porous Media

PI: Dr. Linda M. Abriola *Institution:* University of Michigan

Publication Type: Journal

Bradford, S. A., Abriola, L. M., & Leij, F. J. (1997). Wettability effects on two- and three- fluid relative permeabilities. Journal of Contam. Hydrol., 28, 171-191.

Bradford, S. A., Abriola, L. M., & Rathfelder, K. M. (1998). Flow and entrapment of dense nonaqueous phase liquids in physically and chemically heterogeneous aquifer formations. Adv. Water Res., 22, 117-132.

Lord, D. L., Demond, A. H., Salehzadeh, A., & Hayes, K. F. (1997). Influence of organic acid solution chemistry on subsurface transport properties. 2. Capillary pressure- saturation. Environ. Sci. Technol., 31, 2052-2058.

Lord, D. L., Hayes, K. F., Demond, A. H., & Salehzadeh, A. (1997). Influence of organic acid solution chemistry on subsurface transport properties. 1. Surface and interfacial tension. Environ. Sci. Technol., 31, 2045-2051.

Publication Type: Other

Lord, D. L. (1999). Influence of organic acid and base solution chemistry on interfacial and transport properties of mixed wastes in the subsurface. Ph.D. dissertation. Department of Civil and Environmental Engineering, The University of Michigan. Ann Arbor, MI.

Publication Type: Paper

Bradford, S. A., & Abriola, L. M. (1998). Entrapment and dissolution of organic liquids in chemically heterogeneous porous media. IAHS Publication no. 250, Groundwater Quality: Remediation and Protection. Tubingen, Germany. 167-172.

Publication Type: Proceeding

Bradford, S. A., Abriola, L. M., & Leij, F. J. (1999, in press). Multi-fluid hydraulic properties for fractional wettability porous media. In Van Genuchten, M. Th., Leij, F. J., & Wu, L. (Eds.), Characterization and Measurement of the Hydraulic Properties for Unsaturated Porous Media, University of California. Riverside, CA.

Bradford, S. A., Abriola, L. M., & Rathfelder, K. M. (1998). Simulated entrapment and dissolution of organic liquids in chemically heterogeneous porous media. In Chrysikopoulos, C. V., Bear, J., & Harmon, T. C. (Eds.), Enviromeet 98-Behavior and Remediation of Nonaqueous Phase Contaminants in the Subsurface. University of California. Irvine, CA. 7-16.

Demond, A.H., Hayes, K. F., Lord, D. L., Desai, F., & Salehzadeh, A. (1999, in press). Impact of organic compound chemistry on capillary pressure relationships of sands. In Van Genuchten, M.Th., Leij, F. J., & Wu, L. (Eds.), Characterization and Measurement of the Hydraulic Properties for Unsaturated Porous Media. University of California. Riverside, CA.

Lord, D. L., Demond, A. H., Hayes, K. F., & Salehzadeh, A. (1999, in press). Effects of surfactant chemistry on interfacial tension, wettability, and capillary pressure in multiphase subsurface waste systems. Transport in Porous Media.

Project: 54681

Title: Dynamics of Coupled Contaminant and Microbial Transport in Heterogeneous Pourous Media

PI: Dr. Ellyn Murphy *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Murphy, E. (1999, in press). The hydrolysis and coarbonate complexation of strontium and calcium in aqueous solution: use of molecular modeling calculations in the development of thermodynamic models. Journal of Chemical Thermodynamics.

Project: 54683

Title: Speciation and Structural Characterization of Plutonium and Actinide-Organic Complexes in Surface and Groundwaters

PI: Dr. Ken O. Buesseler *Institution:* Woods Hole Oceanographic Institute

Publication Type: Presentation

Dai, M., et al. (1998, May). Size fractionated Pu isotopes in the ocean, a pond and groundwater. AGU Spring Meeting, Boston, MA. EOS, 79(17), 138.

Dai, M., et al. (1999, May). Isotopic composition, speciation and mobility of Pu in the groundwater at DOE Savannah River Site. AGU Spring meeting. Boston, MA.

Dai, M.H., et. al. (1998, July 27- 30). Size fractionated Pu isotopes in surface and subsurface waters. American Chemical Society DOE Environmental Management Science Program Workshop. Chicago, IL.

Repeta, D.J., Quan, T. M., Aluwihare, L. I., & Accardi, A. (1999). Dissolved organic matter in fresh and marine waters. Amer. Soc. Limnol. Oceanogr. Annual meeting. Santa Fe, NM.

Project: 54684

Title: Mechanism Involved in Trichloroethylene-Induced Liver Cancer: Importance to Environmental Cleanup

PI: Dr. Richard J. Bull *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Kato-Weinstein, J., Lingohr, M. K., Thrall, B. D., & Bull, R. J. (1998). Effects of dichloroacetate on carbohydrate metabolism in B6C3F1 mice. Toxicology 130,141-154

Lingohr, M. K., Thrall, B. D., & Bull, R. J. (1999, in press). Serum insulin levels and differential insulin receptor expression in livers and liver tumors of mice treated with dichloroacetate (DCA). Toxicol. Appl. Pharmacol.

Merdink, J. L., Gonzalez-Leon, A., Bull, R. J., & Schultz, I. R. (1998). The extent of dichloroacetate formation from trichloroethylene, chloral hydrate, trichloroacetate, and trichloroethanol in B6C3F1 mice. Toxicological Sciences 45, 33-41.

Schultz, I. R., Merdink, J. L., Gonzalez-Leon, A., & Bull, R. J. (1999, in press). Comparative toxicokinetics and metabolism of chlorinated and brominated haloacetates in F344 rats. Toxicol. Appl. Pharmacol.

Stauber, A. J., Bull, R. J., & Thrall, B. D. (1998). Dichloroacetate and trichloroacetate promote clonal expansion of anchorage-independent hepatocytes, in vivo and in vitro. Toxicol. Appl. Pharmacol. 150, 287-294.

Publication Type: Poster

Bull, R. J., Minard, K., Sasser, L.B., Lingohr, M. K., & Wind, R.A. (1999). Dichloroacetate-induced liver tumors cease growing on removal of treatment: Result of an insulin-sensitive phenotype? AACR Proceedings 40, 3321

Publication Type: Presentation

Gonzalez-Leon, A., Merdink, J. L., Schultz, I. R., & Bull, R. J. (1998). Dichloroacetate auto-inhibits its degradation in the cytosol. Society of Toxicology, 37th Annual Meeting #426.

Kato-Weinstein, J., Thrall, B. D., & Bull, R. J. (1998). The effect of haloacetates on carbohydrate metabolism in B6C3F1 mice. Society of Toxicology, 37th Annual Meeting #308.

Lingohr, M. K., Thrall, B. D., & Bull, R. J. (1998). Dichloroacetate (DCA) affects proteins involved in insulin signaling in mouse liver cells. Society of Toxicology, 37th Annual Meeting #61.

Merdink, J. L., Schultz, I. R., & Bull, R. J. (1998). Formation of dichloroacetic acid in B6C3F1 mice from trichloroethylene or its metabolites. Society of Toxicology, 37th Annual Meeting #1621.

Mounho, B. J. & Thrall, B. D. (1998). Tumor promotion by peroxisome proliferators may involve the activation of mitogenic activated protein kinases (ERK1/ERK2). Society of Toxicology, 37th Annual Meeting #51.

Orner, G. A., et. al. (1998). Effects of trichloroacetate (TCA) and dichloroacetate (DCA) on H-ras in male B6C3F1 mice. Society of Toxicology, 37th Annual Meeting #60.

Schultz, I. R., Gonzalez-Leon, A., Merdink, J. L., & Bull, R. J. (1998). Comparative toxicokinetics and metabolism of halo-acetic acids in F344 rats. Society of Toxicology, 37th Annual Meeting #1045.

Stauber, A. J., Bull, R. J., & Thrall, B. D. (1998). Dichloroacetate and trichloroacetate promote clonal expansion of anchorage-independent hepatocytes. Society of Toxicology, 37th Annual Meeting #62.

Publication Type: Proceeding

Bull, R. J., Minard, K., Sasser, L. B., Lingohr, M. K., & Wind, R. A. (1999). Dichloroacetate-induced liver tumors cease growing on removal of treatment: Result of an insulin-sensitive phenotype? AACR Proceedings 40, 3321.

Project: 54691

Title: Radiation Effects on Materials in the Near-Field of Nuclear Waste Repository
PI: Dr. Lu-Min Wang *Institution:* University of Michigan

Publication Type: Journal

Gu, B. X., Wang, L. M., & Ewing, R. C. (1999, in press). The effect of amorphization on the Cs ion exchange and retention capacity of zeolite-NaY. Journal of Nuclear Materials.

Wang, S. X., Wang, L. M., & Ewing, R. C. (1999, in press). Electron and ion irradiation of zeolites. Journal of Nuclear Materials.

Wang, S. X., Wang, L. M., & Ewing, R. C. (1999, in press). Electron and ion irradiation of zeolites. Journal of Nuclear Materials.

Publication Type: Proceeding

Wang, S. X., Wang, L. M., & Ewing, R. C. (1999, in press). Electron irradiation of zeolites. Proceedings of the Materials Research Society.

Project: 54716

Title: Polyoxometalates for Radioactive Waste Treatment
PI: Dr. Michael T. Pope *Institution:* Georgetown University

Publication Type: Journal

Dickman, M. H., Gama, G. J., Kim, K. -C., & Pope, M. T. (1996). The structures of europium(III)- and uranium(IV) derivatives of [P 5 W 30 O 110] 15- . Evidence for Cryptohydration. J.Cluster Sci., 7, 67-583.

Kim, K. -C. & Pope, M. T. (1999, in press). Cation-directed structure changes in polyoxometalate chemistry. Equilibria between isomers of bis(9-tungstophosphatodioxouranate(VI)) complexes. J. Am. Chem. Soc.

Müller, A., Peters, F., Pope, M. T., & Gatteschi, D. (1998). Polyoxometalates: Very large structures - nanoscale magnets. Chem. Rev. 98, 239-271.

Pope, M. T., Wei, X., Wassermann, K., & Dickman, M. H. (1998). New developments in the chemistry of heteropolytungstates of rhodium and cerium. C. R. Acad. Sci., 1, Ser. IIc, 297-304.

Wassermann, K., Dickman, M. H., & Pope, M. T. (1997). Self-assembly of supramolecular polyoxometalates. The compact, water-soluble heteropolytungstate anion [As III 12 Ce III 16 (H 2 O)36 W 148 O 524] 76ÿ. Angew. Chem. 109, 1513-1516.

Publication Type: Other

Pope, M. T., Creaser, I. I., & Heckel, M. C. (1997, Apr. 8). Compounds and methods for separation and molecular encapsulation of metalIons. U.S. Patent 5,618,472.

Project: 54724

Title: Synthesis of New Water-Soluble Metal-Binding Polymers: Combinatorial Chemistry Approach
PI: Dr. Barbara F. Smith *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Colletti, L. & Havrilla, G. (1999). Trace element detection with micro-x-ray fluorescence. Advances in X-Ray Analysis, 44.

Kizer, D. E., Miller, R. B., & Kurth, M. J. (1999). Fused pyrazolo heterocycles: intramolecular [3+2]-nitrile oxide cycloadditions applied to syntheses of pyrazolo[3,4-g][2,1]dihydrobenzoisoxazol(in)es. Tetrahedron Letters, 40, 3535-38.

Publication Type: Proceeding

Smith, B. F., Robison, T. W., & Jarvinen, G. D. (1998). Water-soluble metal-binding polymers with ultrafiltration: A technology for the removal, concentration, and recovery of metal ions from aqueous streams. In Rogers, R., Bond, A., & Dietz, M. (Eds.), ACS Symposium Series volume, Advances in Metal Ion Separation and Preconcentration, Chap. 20, 294-330.

Song, J., Corrales, L. R., & Jónsson, H. (1999, in press). Exploring the excited states of vacancy defects in silica. In Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Project: 54735

Title: Development of Inorganic Ion Exchangers for Nuclear Waste Remediation
PI: Dr. Abraham Clearfield *Institution:* Texas A&M University

Publication Type: Journal

Khainakov, S. A., et. al. (1999). Hydrothermal synthesis and characterization of alkali metal titanium silicates. Journal of Materials Chem. 9, 269-272.

Pertierra, P., Salvado, M. A., Garcia-Granda, S., Bortun, A. I., & Clearfield, A. (1999). Neutron powder diffraction study of Ti2(OH)2OSiO4.1.5H2O. Inorganic Chem., 38(11), 2563-2566.

Poojary, D. M., Zhang, B., & Clearfield, A. (1998). Synthesis and structures of barium arylbisphosphonates derived from x-ray powder data. Anales de Quimica Int. Ed., 94, 401-405.

Sylvester, P. & Clearfield, A. (1999). The removal of strontium from simulated Hanford tank wastes containing complexants. Separation Science and Technology, 34(13), 2539-2551.

Sylvester, P., Clearfield, A., & Diaz, R. J. (1999). Pillared montmorillonites: cesium-selective ion-exchange materials. Science and Technology, 34(12), 2293-2305.

Trobajo, C., et. al. (1999). Hydrothermal synthesis and ion exchange properties of the novel framework sodium and potassium niobium silicates. Solvent Extraction and Ion Exchange, 17(3), 649-675.

Project: 54741

Title: Characterization of Contaminant Transport Using Naturally-Occurring U-Series Disequilibria

PI: Dr. Michael T. Murrell *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Luo, S., Ku, T. L., Roback, R., Murrell, M., & McLing, T. (1999, Aug. 21-26). Uranium-series disequilibria in groundwater: Assessing radionuclide migration. 9th International Conference on Isotope Geology, Cosmochemistry and Geochronology. Beijing, China.

Luo, S., Ku, T. L., Roback, R., Murrell, M., & McLing, T. (1998, Dec. 6-10). Assessing in-situ radionuclide transport based on uranium-series disequilibrium in groundwater. Fall AGU Meeting. San Francisco, CA. EOS Trans. Amer. Geophys. Un. 79, F354.

Roback, R. C., et. al. (1997). Groundwater mixing, flow-paths and water/rock interaction at INEEL: Evidence from uranium isotopes. Geological Society of America, Abstracts with Programs, 29(6).

Roback, R. C., et. al. (1998, Dec. 6-10). Uranium and thorium series isotopes in fractured rocks at the INEEL. Fall AGU Meeting. San Francisco, CA. EOS Trans. Amer. Geophys. Un. 79, F343.

Project: 54765

Title: Enhanced Sludge Processing of HLW: Hydrothermal Oxidation of Chromium, Technetium, and Complexants by Nitrate

PI: Dr. Stephen J. Buelow *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Goemans, M. G. E., Funk, T. J., Sedillo, M. A., Buelow, S. J., & Anderson, G. K. (1997). Electrical conductances of aqueous solutions of inorganic nitrates ate 25-505_C and 100-490 bar,î. Journal of Supercritical Fluids 11, 61-72.

Publication Type: Poster

Buelow, S. J. (No date given). Dissolution of chromium oxide under hydrothermal conditions. AIChE National Spring Meeting.

Project: 54770

Title: New Anion-Exchange Resins for Improved Separations of Nuclear Materials

PI: Dr. Mary E. Barr *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Marsh, S. F., Jarvinen, G. D., & Bartsch, R. A. (1997). New bifunctional anion-exchange resins for nuclear waste treatment. Reactive Polymers, 35, 75-80.

Marsh, S. F., Jarvinen, G. D., Bartsch, R. A., Nam, J., & Barr, M. E. (1998). New bifunctional anion-exchange resins for nuclear waste treatment-II. J. Radioanal. Nucl. Chem., 235, 37-40.

Publication Type: Presentation

Barr, M. E., Jarvinen, G. D., Marsh, S. F., & Bartsch, R. A. (1997, Apr. 13). Development of anion-exchange resins for separations of actinides. Abstracts of Papers of the American Chemical Society, 213(pt.2), 73-IEC.

Barr, M. E., Jarvinen, G. D., Moody, E. W., & Vaughn, R. B. (1998, Aug. 23). Sorption of Pu(IV) by soluble anion-exchange polymers. Abstracts of Papers of the American Chemical Society, 216(pt.2), 88-NUCL, & 216(pt.1), 5-TECH.

Barr, M. E., Jarvinen, G. D., Schulte, L. D., Stark, P. C., & Chamberlin, R. M. (1999, Mar. 21). Americium separations from complex mixtures using anion exchange. Abstracts of Papers of the American Chemical Society, 217, 019-IEC.

Bartsch, R. A., et. al. (1999, Mar. 21). Sorption of Pu(IV) from nitric acid by bifunctional anion-exchange resins. Abstracts of Papers of the American Chemical Society, 217, 125-IEC.

Marsh, S. F., Jarvinen, G. D., Bartsch, R. A., Nam, J., & Barr, M. E. (1997, Apr.). New bifunctional anion-exchange resins for nuclear waste treatment. Marc IV conference on Radioanalytical Chemistry, Kona, HI.

Moody, E. W., Barr, M. E., & Jarvinen, G. D. (1999). QSAR of distribution coefficients for actinide hexanitrato complexes. Abstracts of Papers of the American Chemical Society, 217(pt.2), 170-NUCL.

Project: 54773

Title: Microstructural Properties of High-Level Waste Concentrates and Gels with Raman and Infrared Spectroscopies

PI: Dr. Stephen F. Agnew *Institution:* Los Alamos National Laboratory

Publication Type: Paper

Agnew, S. F. (1999, March 1). Raman scattering, ingrared absoption, and telative humidity of mono- and trisodium aluminate. I&EC Division Symposium on Radioactive and Hazardous Waste Forms, National Meeting of the American Chemical Society.

Publication Type: Presentation

Agnew. S. F. (1999, March 11). Microsturctural properties of high-level waste concentrates and gels with raman and infrared spectroscopies. Cross-Cut Workshop.

Project: 54790

Title: Microbial Mineral Transformations at the Fe(II)/Fe(III) Redox Boundary for Solid Phase Capture of Strontium and Other Metal/Radionuclide Contaminants

PI: Dr. F. Grant Ferris *Institution:* University of Toronto

Publication Type: Journal

Howell, J. R., Donahoe, R. J., Roden, E. E., & Ferris, F. G. (1998). Effects of microbial iron oxide reduction on pH and alkalinity in anaerobic bicarbonate-buffered media: Implications for metal mobility. Mineralogical Magazine, 62A, 657-658.

Publication Type: Other

Howell, J. R. (1998). Effects of microbial Fe(III) oxide reduction on pH, DIC, and carbonate mineral formation: Implications for metal mobility. M. S. Thesis, Department of Geology, University of Alabama. Tuscaloosa, AL.

Publication Type: Presentation

Maurice, P.A., Warren, L. A., & Ferris, F. G. (1998). Calcite precipitation by B. pasteurei: AFM imaging of microbial-mineral interactions. Geological Society of America Annual Meeting. Toronto, Canada.

Parmar, N., Warren, L. A. & Ferris, F. G. (1998). Solid phase capture of strontium by the iron reducing bacteria Shewenella alga. Geological Society of America Annual Meeting. Toronto, Canada.

Small, T.D., Warren, L. A., & Ferris, F. G. (1998). Strontium sorption to bacterial and Fe oxide surfaces. Geological Society of America Annual Meeting. Toronto, Canada.

Warren, L. A., Parmar, N., & Ferris, F. G. (1998). Strontium, uranyl, and copper incorporation in bacterially mediated calcite precipitation. Geological Society of America Annual Meeting. Toronto, Canada.

Publication Type: Proceeding

Warren, L. A. & Ferris, F. G. (1998). Solid phase partitioning of uranium and copper in the presence of HFO and bacteria. In Arehart, G. B. & Hulston, J. R. (Eds.), Proceedings of the 9th International Symposium on Water Rock Interaction WRI-9. Balkema, Rotterdam. 115-117.

Project: 54834

Title: An Investigation of Homogeneous and Heterogeneous Sonochemistry for Destruction of Hazardous Waste

PI: Dr. Inez Hua *Institution:* Purdue University

Publication Type: Presentation

Hua, I. (1999, Feb.). The use of ultrasonic irradiation in environmental engineering processes. Borchardt Conference, The University of Michigan. Ann Arbor, MI.

Pfalzer, U. & Hua, I. (1997, Nov. 9). Sonochemical degradation of carbofuran in a parallel-plate near-field acoustical processor. 20th Annual Midwest Environmental Chemistry Workshop, Indiana University. Bloomington, IN.

Schramm, J. & Hua, I. (1997, Sept.). Degradation of dichlorvos by sonolysis. American Chemical Society Meeting. Las Vegas, NV.

Zhang, G. & Hua, I. (1998, Mar.). Destruction of polychlorinated biphenyls in acoustically cavitating systems. American Chemical Society Meeting. Dallas, TX.

Project: 54837

Title: Phytoremediation of Ionic and Methyl Mercury Pollution
PI: Dr. Richard B. Meagher *Institution:* University of Georgia

Publication Type: Journal

Heaton, A. C. P., Rugh, C. L., Wang, N. -J., & Meagher, R. B. (1998). Phytoremediation of mercury and methylmercury polluted soils using genetically engineered plants. J. Soil Contam. 7, 497-509.

Heaton, A. C. P., Rugh, C. L., Wang, N. -J., & Meagher, R. B. (1998). Phytoremediation of mercury and methylmercury polluted soils using genetically engineered plants. J. Soil Contam. 7: 497-509.

Rugh, C. L., Gragson, G. M., & Meagher, R. B. (1998). Toxic mercury reduction and remediation using transgenic plants with a modified bacterial gene. Hort. Sci. 33, 12-15.

Rugh, C. L., Gragson, G. M., & Meagher, R. B. (1998). Toxic mercury reduction and remediation using transgenic plants with a modified bacterial gene. Hort. Sci. 33, 12-15.

Rugh, C. L., Senecoff, J. F., Meagher, R. B., & Merkle, S. A. (1998). Development of transgenic yellowpoplar for mercury phytoremediation. Nature Biotech. 16, 925-928.

Rugh, C. L., Senecoff, J. F., Meagher, R. B., & Merkle, S. A. (1998). Development of transgenic yellowpoplar for mercury phytoremediation. Nature Biotech. 16, 925-928.

Publication Type: Other

Rugh, C. L., Bizily, S. P., & Meagher, R. B. (1999). Phytoremediation of environmental mercury pollution. In Ensley, B. & Raskin, I. (Eds.), Phytoremediation of toxic metals: Using plants to clean-up the environment. Wiley and Sons, New York, NY.

Rugh, C. L., Bizily, S. P., & Meagher, R. B. (1999, in press). Phytoremediation of environmental mercury pollution. In Ensley, B. & Raskin, I. (Eds.), Phytoremediation of toxic metals: Using plants to clean-up the environment. Wiley and Sons, New York, NY.

Publication Type: Paper

Meagher, R. B. & Rugh, C. L. (1996). Phytoremediation of heavy metal pollution: Ionic and methylmercury. OECD Biotechnology for Water Use and Conservation Workshop. Organization for Economic Co-Operation and Development. Cocoyoc, Mexico. 305-321.

Meagher, R. B. (1998). Phytoremediation: An affordable, friendly technology to restore marginal lands in the twenty-first century. Plants and Population: Is there time? Natl. Acad. Sci. Colloquium. Irvine, CA.

Publication Type: Proceeding

Bizily, S., Rugh, C. L., Summers, A. O., & Meagher, R. B. (1999). Phytoremediation of methylmercury pollution: MerB expression in Arabidopsis thaliana confers resistance to organomercurials. Proc. Natl. Acad. Sci. USA 96, 6808-6813.

Bizily, S., Rugh, C. L., Summers, A. O., & Meagher, R. B. (1999, in press). Phytoremediation of methylmercury pollution: merB expression in Arabidopsis thaliana confers resistance to organomercurials. Proc. Natl. Acad. Sci. USA.

Meagher, R. B. & Rugh, C. L. (1996). Phytoremediation of heavy metal pollution: Ionic and methylmercury. OECD Biotechnology for Water Use and Conservation Workshop. Organization for Economic Co-Operation and Development. Cocoyoc, Mexico. 305-321.

Meagher, R. B., Rugh, C. L., Kandasamy, M. K., Gragson, G., & Wang, N. J. (1998). Engineered phytoremediation of mercury pollution in soil and water using bacterial genes. In Ishndar, I. K., Hardy, S. E., Chang, A. C., & Pierzynski, G. M. (Eds.), Fourth International Conference on the Biogeochemistry of Trace Elements. Ann Arbor Press, Inc. Berkeley, CA. 653-654.

Meagher, R.B., Rugh, C. L., Kandasamy, M. K., Gragson, G., & Wang, N. -J. (1998). Engineered phytoremediation of mercury pollution in soil and water using bacterial genes. In Ishndar, I. K., Hardy, S. E., Chang, A. C., & Pierzynski, G. M. Fourth International Conference on the Biogeochemistry of Trace Elements pp. Ann Arbor Press, Inc. Berkeley, CA. 203-221.

Rugh, C. L., et. al. (1996). Mercuric ion reduction and resistance in transgenic Arabidopsis thaliana plants expressing a modified bacterial merA gene. Proc. Natl. Acad. Sci. USA 93, 3182-3187.

Rugh, C. L., et. al. (1996). Mercuric ion reduction and resistance in transgenic Arabidopsis thaliana plants expressing a modified bacterial merA gene. Proc. Natl. Acad. Sci. USA 93, 3182-3187.

Project: 54847

Title: Photocatalytic and Chemical Oxidation of Organic Compounds in Supercritical Carbon Dioxide

PI: Dr. Daniel M. Blake *Institution:* National Renewable Energy Laboratory

Publication Type: Journal

Jacoby, W. A., et al. (1996). Heterogeneous photocatalysis for control of volatile organic compounds in indoor air. J. Air Waste Manage. Assoc., 46(9), 891-8.

Project: 54864

Title: Supramolecular Chemistry of Selective Anion Recognition for Anions of Environmental Relevance

PI: Dr. Kristin Bowman-James *Institution:* University of Kansas

Publication Type: Journal

Mason, S., Clifford, T., Seib, L., Kuczera, K., & Bowman-James, K. (1998). Unusual encapsulation of two nitrates in a single bicyclic cage. J. Am. Chem. Soc. 120, 8899-8900.

Wiórkiewicz-Kuczera, et. al. (1999, in press). Solid state to solution: Crystal structure and molecular dynamics. In Simulations of a Polyammonium Nitrate Host, New J. Chem.

Publication Type: Other

Bianchi, A., Bowman-James, K., & García-Espana, E. (Eds.). (1997), Supramolecular Chemistry of Anions, Wiley-VCH. New York, NY.

Wiórkiewicz-Kuczera, J. & Bowman-James, K. (1997). Anion Binding Receptors: Theoretical Studies. In Bianchi, A., Bowman-James, K., & García-España, E. (Eds.), Supramolecular Chemistry of Anions. Wiley-VCH, New York, NY. 335-354.

Project: 54898

Title: Molecular Dissection of the Cellular Mechanisms Involved in Nickel Hyperaccumulation in Plants

PI: Dr. David E. Salt *Institution:* Northern Arizona University

Thlaspi Goesingense growing in its native ultramafic habitat near Redschlag/Austria. The Northern Arizona University team is investigating, at the molecular level, the role of histidine biosynthesis in byperaccumulation in *Thlaspi goesingense*. [see Project #54898]

Publication Type: Journal

Krämer, U., Smith, R. D., Wenzel, W., Raskin, I., & Salt, D. E. (1997). The role of nickel transport and tolerance in nickel hyperaccumulation by Thlaspi goesingense Hálácsy. Plant Physiol, 115, 1641-1650.

Persans, M., Xiange,Y., Patnoe, J. M. M. L., Krämer, U., & Salt, D. E. (1999, in press). Molecular dissection of histidine's role in nickel hyperaccumulation in Thlaspi goesingense (Hálácsy). Plant Physiology.

Persans, M., Yan, X., Smith, R., & Salt, D. E. (1998). Cloning of two cDNA's from the Ni hyperaccumulator Thlaspi goesingense: Histidinol dehydrogenase (Accession No. AF023141) and imidazolglycerol-phosphate dehydratase (Accession No. AF023140), two enzymes in the histidine biosynthetic pathway. Plant Physiol Plant Gene Register, 117, 332.

Salt, D. E., Prince, R. C., Baker, A. J. M., Raskin, I., Pickering, I. J. (1999). Zinc ligands in the metal hyperaccumulator Thlaspi caerulescens as determined using X-ray absorption spectroscopy. Environmental Science and Technology 33, 713-717.

Salt, D. E., Prince, R. C., Baker, A. J. M., Raskin, I., & Pickering, I. J. (1999). Zinc ligands in the metal hyperaccumulator Thlaspi caerulescens as determined using X-ray absorption spectroscopy. Environ Sci Technol 33, 713-717.

Salt, D. E., Smith, R. D., & Raskin, I. (1998). Phytoremediation. Ann Rev Plant Physiol Plant Mol Biol, 49, 643-668.

Publication Type: Other

Salt, D. E. (1999, in press). Phytoextraction: Present applications and future promise. In Wise, D. L., Trantolo, D. J., Inyang, H. I., & Cichon, E. J. (Eds.), Remediation of Hazardous Waste Contaminated Soils, 2nd Edition, Marcel Dekker, Inc.

Salt, D. E. (1999, in press). Phytoextraction: Present applications and future promise. In Wise, D. L., Trantolo, D. J., Inyang, H. I., & Cichon, E. J. (Eds.), Remediation of Hazardous Waste Contaminated Soils, 2nd Edition. Marcel Dekker, Inc.

Salt, D. E., & Baker, A. J. M. (1999, in press). Phytoremediation of metals. In Rehm, H. -J. & Reed, G. (Eds.),Biotechnology 2nd Edition, Wiley-VCH. New York, NY.

Salt, D. E., & Krämer, U. (1999, in press). Mechanisms of metal hyperaccumulation in plants. In Ensley, B. D. & Raskin, I. (Eds.), Phytoremediation of Toxic Metals: Using Plants to Clean-Up the Environment, Chapter 13, John Wiley & Sons, Inc., New York, NY.

Salt, D. E., Kato, N., Krämer, U., Smith, R. D. & Raskin, I. (1999). The role of root exudates in nickel hyperaccumulation and tolerance in accumulator and non-accumulator species of Thlaspi. In Terry, N. & García-España, X. (Eds.), Phytoremediation of Contaminated Soil and Water, Chapter 10, CRC Press LLC. Boca Raton, FL. 189-200.

Salt, D. E., Kato, N., Krämer, U., Smith, R. D. & Raskin, I. (1999, in press). The role of root exudates in nickel hyperaccumulation and tolerance in accumulator and non-accumulator species of Thlaspi. In Terry, N., Bañuelos, G. S. (Eds.), Phytoremediation of Contaminated Soil and Water, Chapter 10, CRC Press LLC, Boca Raton, FL.191-202

Wenzel, W., Salt, D. E., Smith, R. D., & Adriano, D. C. (1999). Phytoremediation: A plant-microbe-based remediation system. In Adriano, D. C., et. al. (Eds.), Bioremediation of Contaminated Soils. American Society of Agronomy Inc., Crop Science Society of America, Inc., Soil Science Society of America, Inc., Madison, Wisconsin. 18, 457-508.

Publication Type: Paper

Special Symposium - Phytoremediation. (1999, Jul. 11-15). Progress towards a molecular understanding of metal hyperaccumulation in plants. 5th International Conference on the Biogeochemistry of Trace Elements. Vienna, Austria.

Publication Type: Presentation

Plenary Address - Phytoremediation as a Clean-Up Technology for the Next Millennium (1999, Jun. 23-25). The Researcher's Perspective - Progress and Bottlenecks. 4th IBC Annual International Conference on Phytoremediation, Toronto, Canada.

Remediation Mini-Symposium. (1999, Jul. 24-28). Towards a molecular understanding of the mechanim of Ni hyperaccumulation in Thlaspi. American Society of Plant Physiologists Annual Meeting. Baltimore, MD.

Project: 54908

Title: Partitioning Tracers for In Situ Detection and Quantification of Dense Non-aqueous Phase Liquids in Groundwater Systems

PI: Dr. Mark L. Brusseau *Institution:* University of Arizona

Publication Type: Journal

Brusseau, M. L., Nelson, N. T., & Costanza, M. S. (1999, in press). Partitioning tracer tests for characterizing immiscible-fluid saturations and interfacial areas in subsurface systems.

Nelson, N. T., et. al. (1999, in press). A gas-phase partitioning tracer method for the in-situ measurement of soil-water content. Water Resour. Res.

Nelson, N. T., Oostrom, M., Wietsma, T. W., & Brusseau, M. L. (1999, in press). The partitioning tracer method for the in-situ measurement of DNAPL saturation: Influence of heterogeneity and sampling method. Environ. Sci. Technol.

Project: 54914

Title: Atmospheric-Pressure Plasma Cleaning of Contaminated Surfaces
PI: Dr. Robert F. Hicks *Institution:* University of California at Los Angeles

Publication Type: Journal

Babayan, S. E., et. al. (1998, in press). Plasma source science and technology.

Jeong, J. Y., et. al. (1998). Plasma source science and technology, accepted for publication in 1998.

Project: 54973

Title: A Novel Energy-Efficient Plasma Chemical Process for the Destruction of Volatile Toxic Compounds
PI: Dr. Lal A. (ORNL) *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Ding, W., McCorkle, D. L., & Pinnaduwage, L. A. (1998). Enhanced formation of negative ions by electron attachment to highly-excited molecules in a flowing afterglow plasma. J. Appl. Phys. 84, 3051.

Ding, W., Pinnaduwage, L. A., Tav, C., & McCorkle, D. L. (1999). The role of high Rydberg states in enhanced o-formation in a pulsed O2 discharge. Plasma Sources Sci. Technol. 8, 384.

Ma, C. Y., McCorkle, D. L., Ding, W., & Pinnaduwage, L. A. (1999, in press). A methodology for direct sampling and gas chromatographic/mass spectral analysis of volatile organic compounds emerging from a low pressure flow-through reaction cell. J. Chromatography.

Ma, C. Y., McCorkle, D. L., Ding, W., & Pinnaduwage, L. A. (1999, in press). A methodology for direct sampling and gas chromatographic/mass spectral analysis of volatile organic compounds emerging from a low pressure. Flow-Through Reaction Cell. J. Chromatography.

McCorkle, D. L., Ding, W. X., Ma, C. Y., & Pinnaduwage, L. A. (1999, in press). Decomposition of benzene in a pulsed glow discharge. Journal of Applied Physics.

McCorkle, D. L., Ding, W. X., Ma, C. Y., & Pinnaduwage, L. A. (1999, in press). Decomposition of benzene in a pulsed glow discharge. Journal of Applied Physics.

McCorkle, D. L., Ding, W., Ma, C. Y., & Pinnaduwage, L. A. (1999). Exploratory studies on a plasma remediation process based on enhanced dissociative electron attachment to highly-excited molecules. J. Phys. D., 32, 46.

Pinnaduwage, L. A., et. al. (1999). Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges. J.Appl. Phys., 85, 7064.

Pinnaduwage, L. A., McCorkle, D. L., & Ding, W. (1997). Enhanced electron attachment to highly excited molecules using a plasma mixing scheme. Appl. Phys. Lett. 71, 3634.

Pinnaduwage, L. A., Tav, C., McCorkle, D. L., & Ding, W. (1999). Temperature dependence of electron attachment to methylene chloride. J. Chem. Phys., 110, 9011.

Publication Type: Presentation

Ding, W., Ma, C. Y., McCorkle, D. L., & Pinnaduwage, L. A. (1998, Jun. 1-4). Decomposition of volatile organic compounds in a positive column glow discharge plasma. Presented at the 25th IEEE International Conference on Plasma Science. Raleigh, NC.

Ding, W., McCorkle, D. L., & Pinnaduwage, L. A. (1998, Jun. 1-4). Enhanced radical formation by electron attachment to highly-excited states of molecules in plasmas. Presented at the 25th IEEE International Conference on Plasma Science. Raleigh, NC.

Ding, W., McCorkle, D. L., Ma, C. Y., & Pinnaduwage, L. A. (1999, Oct. 5-8). Dissociation of benzene in a pulsed glow discharge. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Ma, C. Y., McCorkle, D. L., Ding, W., & Pinnaduwage, L. A. (1998, May 31 - Jun. 4). A methodology for direct sampling of volatile organic compounds emerging from a low-pressure, flow-through reaction cell for subsequent GC-GC/MS analysis. Presented at the 46th ASMS Conference on Mass Spectrometry and Allied Topics. Orlando, FL.

McCorkle, D. L. & Pinnaduwage, L. A. (1997, Oct. 6-9). Destruction of CH2Cl2 using a glow discharge scheme. 50th Annual Gaseous Electronics Conference. Madison, WI.

Pinnaduwage, L. A. (1997, Jun. 29 - Jul. 2). Implications of electron attachment to highly-excited states in pulsed power discharges. 11th IEEE Pulsed Power Conference. Baltimore, MA.

Pinnaduwage, L. A., Ding, W., & McCorkle, D. L. (1999, Oct. 5-8). Negative ion formation in pulsed plasmas. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Pinnaduwage, L. A., Ma, C. Y., McCorkle, D. L., & Ding, W. (1998, Jul. 27-30). A novel energy-efficient plasma chemical process for the destruction of volatile toxic compounds. Presented at the Environmental Management Science Program Workshop. Chicago, IL.

Tav, C. & Pinnaduwage, L. A. (1999, Oct. 5-8). Dissociative electron attachment to laser-excited benzene. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Publication Type: Proceeding

Pinnaduwage, L. A. (1997). Implications of electron attachment to highly-excited states in pulsed power discharges. In Cooperstein, G. & Vitkovitsky, I. (Eds.), Digest of Technical Papers of the 11th IEEE Pulsed Power Conference. IEEE Publishing Services. New York, NY. 1048-1053.

Pinnaduwage, L. A., Datskos, P. G., Ding, W. X., & McCorkle, D. L. (1999, in press). Enhanced electron attachment to highly-excited states of molecules: Implications for plasma processing discharges. Proceedings of the 1998 International Congress on Plasma Physics.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1999, in press). Enhanced electron attachment to superexcited Rydberg states of molecular hydrogen using a plasma mixing scheme. Proceedings of the 1998 International Congress on Plasma Physics.

Project: 54996

Title: Ionizing Radiation Induced Catalysis on Metal Oxide Particles
PI: Dr. Michael A. Henderson *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Epling, W. S., Peden, C. H. F., Henderson, M. A., & Diebold, U. (1998). Evidence for oxygen adatoms on TiO2(110) resulting from O2 dissociation at vacancy sites. Surf. Sci. 412-413, 333.

Henderson, M. A., Epling, W. S., Perkins, C. L., Peden, C. H. F., & Diebold, U. (1999, in press). Interaction of molecular oxygen with the vacuum annealed TiO2(110) surface: Molecular and dissociative channels. J. Phys. Chem.

Henderson, M. A., Oreto-Tapia, S., & Castro, M. E. (1998). Electron induced decomposition of CH3OH on the vacuum annealed surface of TiO2(110). Surf. Sci. 412-413, 252.

Herman, G. S., Henderson, M A., Starkweather, K. A., & McDaniel, E. P. (1999, in press). Mass- spectrometry of recoiled ions and secondary ion mass spectrometry investigation of Y-stabilized ZrO2(100) and (110). J. Vac. Sci. Technol. A.

Su, Y., et. al. (1998). Gamma-ray destruction of EDTA catalyzed by titania. J.

Adv. Oxid. Technol. 3, 63.

Taylor, D. P., Simpson, W. C., Knutsen, K., Henderson, M. A., & Orlando, T. M. (1998). Photon stimulated desorption of cations from yttria-stabilized cubic ZrO2(100). Appl. Surf. Sci. 102, 4536.

Publication Type: Presentation

Henderson, M. A. (1998). Coadsorption studies with water: A small step toward understanding the surface chemical and photochemical properties of TiO2. Invited presentation at the 45th National Symposium of the American Vacuum Society. Baltimore, MA.

Henderson, M. A. (1998). Coadsorption studies with water and oxygen: A small step toward understanding the surface chemical and photochemical properties of TiO2. Invited presentation at the Department of Chemistry, University of Puerto Rico. Mayaquez, Puerto Rico.

Henderson, M. A. (1998). Ionizing radiation induced catalysis: Radiocatalytic degradation of organic contaminants in TiO2 suspensions. Invited presentation at the Notre Dame Radiation Laboratory, University of Notre Dame. South Bend, IN.

Henderson, M. A. (1999). Activation of molecular oxygen on TiO2(110) by reaction with bridging hydroxyls. First International Workshop on Oxide Surfaces. Elmau, Germany.

Su, Y. (1999, May 2-6). Radiocatalytic and photocatalytic studies of oxidation of organics and reduction of water. The 195th Meeting of the Electrochemical Society, Seattle, WA.

Su, Y. (1999, May 24-28). Radiocatalytic and photocatalytic studies of metal ion reduction and water cleavage into hydrogen. The 5th International Conference on Advanced Oxidation Technologies for Water and Air Remediation, Albuquerque, NM.

Project: 55011

Title: Surface and Borehole Electromagnetic Imaging of Conducting Contaminant Plumes

PI: Dr. James G. Berryman *Institution:* Lawrence Livermore National Laboratory

Publication Type: Journal

Borcea, L., Berryman, J. G., & Papanicolaou, G. C. (1999). Matching pursuit for imaging high contrast conductive media. Inverse Problems, Vol. 15, 811—849.

Dorn, O., Bertete-Aguirre, H., Berryman, J. G., & Papanicolaou, G. C. (1999, in press). A nonlinear inversion method for 3D-electromagnetic imaging using adjoint fields. Inverse Problems.

Publication Type: Paper

Berge, P. A. & Berryman, J. G. (1999, Mar. 24-27). Developing rock physics algorithms for velocity-porosity relations with environmental geophysics applications. Invited presentation at the Fifth SIAM Conference on Mathematical and Computational Issues in the Geosciences. San Antonio, TX.

Berge, P. A., Berryman, J. G., Bonner, B. P., Roberts, J. J., & Wildenschild, D. (1999, Mar. 14-18). Comparing geophysical measurements to theoretical estimates for soil mixtures at low pressures. Invited presentation in the 1999 Conference Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Oakland, CA. 465—472.

Buettner, H. M. & Berryman, J. G. (1999, Mar. 14-18). An electromagnetic induction tomography field experiment at Lost Hills, CA. Invited presentation at the 1999 Conference Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP), Oakland, CA. 663—672.

Champagne II, N. J., Berryman, J. G., Buettner, H. M., Grant, J. B. & Sharpe, R. M. (1999, Mar. 14-18). A finite-difference frequency-domain code for electromagnetic induction tomography. Poster and paper in 1999 Conference Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP), Oakland, CA. 931—940.

Publication Type: Patent

Berryman, J. G. (1998, Dec. 8). Robust discrimination of porosity and fluid saturation using seismic velocity analysis. Patent disclosure IL-10437.

Berryman, J. G. (1998, Nov. 6). Joint inversion of electrical and electromagnetic tomography data for mapping saturation level and connectivity of conducting fluids underground. Patent disclosure IL-10412.

Publication Type: Presentation

Berryman, J. G. (1997, Aug. 25-29). Challenges for computational physics in underground imaging of electrically conducting contaminant plumes. Invited presentation P2.03 in special session on Geological Phenomena at the International Conference on Computational Physics. American Physical Society, Division of Computational Physics. Santa Cruz, CA.

Berryman, J. G. (1998, Oct. 19-23). Underground imaging of electrically conducting plumes. Invited presentation at the International Advanced Studies Institute, First International Symposium on Detection and Analysis of Subsurface Objects and Phenomena, Naval Postgraduate School. Monterey, CA.

Berryman, J. G., Berge, P. A. & Bonner, B. P. (1999, Nov. 4). Role of lambda-diagrams in estimating porosity and saturation from seismic velocities. Invited presentation at SEG, Houston, TX.

Publication Type: Proceeding

Berge, P. A., Roberts, J. J., Berryman, J. G., & Wildenschild, D. (1998, Jul. 27-30). Joint inversion of geophysical data for site characterization and restoration monitoring. Abstract #188 in Proceedings of Environmental Sciences Management Workshop. Chicago, IL. 378—380.

Berryman, J. G. (1998, Jul. 27-30). Surface and borehole electromagnetic imaging of conducting contaminant plumes. Abstract #189 in Proceedings of Environmental Sciences Management Workshop. Chicago, IL. 380—382.

Berryman, J. G., Champagne II, N. J., & Buettner, H. M. (1999, Oct. 27-29). A 3D finite-difference frequency-domain code for electromagnetic induction tomography. Proceedings of the Second International Symposium on Three Dimensional Electromagnetics, University of Utah. Salt Lake City, UT.

Project: 55013

Title: Biofiltration of Volatile Pollutants: Engineering Mechanisms for Improved Design, Long-term Operation, Prediction and Implementation

PI: Dr. Brian H. Davison *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Barton, J. W., Davison, B. H., Klasson, K. T., & Gable III, C. C. (1999). Estimation of mass transfer of kinetics in operating trickle bed bioreactors for removal of VOCs. Environmental Progress, 181-5.

Barton, J. W., Davison, B. H., Klasson, K. T., & Gable III, C. C. (1999). Estimation of mass transfer and kinetics in operating trickle-bed bioreactors for removal of VOCs. Environ. Prog. 18,1-5.

Barton, J. W., Hartz, S., Klasson, K. T., & Davison, B. H. (1998). Microbial removal of alkanes from dilute gaseous waste streams: Mathematical modeling of advanced bioreactor systems. J. Chem. Technol. Biotechnol. 72,93-98.

Publication Type: Proceeding

Barton, J. W., Zhang, X. S., Davison, B. H., & Klasson, K. T. (1999, Oct. 22-23). Predictive mathematical modeling of trickling bed biofilters. Proceedings of the 1998 USC-TRG Conference on Biofiltration. Los Angeles, CA.

Barton, J. W., Zhang, X. S., Klasson, K. T., & Davison, B. H. (1998, Jun.). Predictive mathematical modeling of trickling bed biofilters for elucidating mass transfer and kinetic effects. Proceedings of the 91st Annual Meeting of the Air and Waste Management Association. San Diego, CA. Paper 98-WAA.13P.

Klasson, K. T., Barton, J. W., & Davison, B. H. (1999, June). Performance of a propane-degrading bacterium. Proceedings of the 92nd Annual Meeting of the Air and Waste Management Association.

Klasson, K. T., Davison, B. H., Barton, J W., & Jacobs, J. E. (1998, Jun.). Removal of chlorinated and nonchlorinated alkanes in a trickling bed biofilter. Proceedings of the 91st Annual Meeting of the Air and Waste Management Association. San Diego, CA. Paper 98-WAA.06P.

Project: 55014

Title: Kinetics and Mechanisms of Metal Retention/Release in Geochemical Processes in Soil

PI: Dr. Robert W. Taylor *Institution:* Alabama A&M University

Publication Type: Journal

Shen, S., Taylor, R. W., Bart, H., & Tu, S. (1999, in press). Equilibrium and spectroscopic studies of lead retention in smectite. Commun. Soil Sci. Plant Analysis.

Publication Type: Presentation

Bleam, W. F., et. al. (1998). Recent advances in understanding the chemistry of Cr(VI), Pb(II) and Hg(II) in soils. Agronomy Abstracts. Baltimore, MD. 36.

Shen, S., Taylor, R. W., Bleam, W. F., & Tu, S. I. (1998). Coupled reduction-sorption of chromate in dithionite-reduced smectites. Agronomy Abstracts. Baltimore, MD. 189.

Szulczewski, M. D., Xia, K., Helmke, P. A., Bleam, W. F., & Taylor, R. W. (1998). Evaluating the reductive capacity of humic substances: Reactions between thiol/thio groups and chromate. Agronomy Abstracts, Baltimore, MD. 38.

Taylor, R. W., Shen, S., Bleam, W. F., & Tu, S. (1999, Jul. 11-15). Chromate removal by dithionite-reduced clays. 5th International Conference on the Biogeochemistry of Trace Elements. Vienna, Austria.

Project: 55031

Title: Genetic Analysis of Stress Responses in Soil Bacteria for Enhanced Bioremediation of Mixed Contaminants

PI: Dr. Kwong-Kwok Wong *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Markillie, L. M., Varnum, S., Hradecky, P., & Wong, K. K. (1999). Targeted mutagenesis by duplication insertion in the radioresistant bacterium Deinococcus radiodrans: Radiation sensitivities of catalase (katA) and superoxide dismutase (sodA) mutants. Journal of Bacteriology, 181, 666-669.

Publication Type: Poster

Wong, K. (1998, Jan 12). Genetic analysis of a catalase mutant of deinococcus radiodurans R1. DOE NAMBIR Workshop.

Publication Type: Presentation

Wong, K. (1997, Oct 12). Genetic analysis of atress responses of deinococcus radiodurans R1. American Society for Microbiology - E. coli and Small Genomes Meeting.

Project: 55033

Title: Characterization of Chemically Modified Hyperthermophilic Enzymes for Chemical Syntheses and Bioremediation Reactions
PI: Dr. Brian H. Davison *Institution:* Oak Ridge National Laboratory

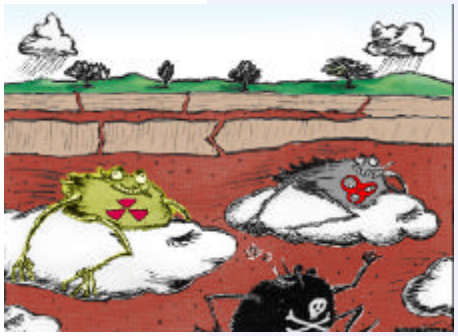
Publication Type: Journal

Kim., C., Woodward, C. A., Kaufman, E. N., & Adams, M. W. W. (1999, in press). Stability and sulfur reduction activity in organic media of hydrogenase from the hyperthermophilic Pyrococcus furiousus. Biotech. Bioeng.

Wang, P., Woodward, C. A., & Kaufman, E. N. (1999, in press). Poly(ethylene glycol)-modified ligninase enhances pentachlorophenol biodegradation in water-solvent mixtures. Biotech. Bioeng.

Project: 55036

Title: Colloid Transport and Retention in Fractured Deposits
PI: Dr. John F. McCarthy *Institution:* Oak Ridge National Laboratory



Mobile colloids in the subsurface environment may alter the transport of contaminants. [see Project #55036]

Publication Type: Paper

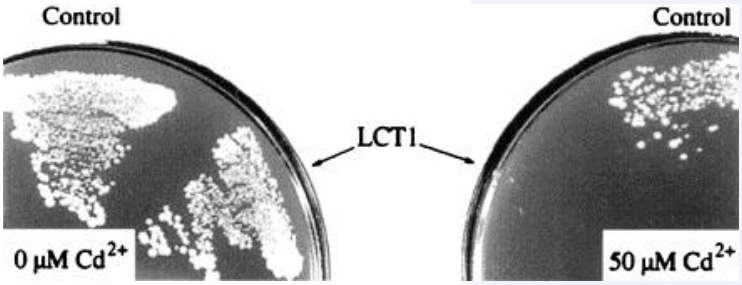
McCarthy, J. F. (1998, May 14). The role of electrostatic attachment of particle transport in fractured shale. Mass Transport in Fractured Aquifers and Aquitards Conference. Copenhagen, Denmark.

Publication Type: Presentation

McCarthy, J. F. (1999, March 21-26). Colloid transport and retention in fractured deposits - Keynote Address. 217th American Chemical Society National Meeting. Anaheim, CA.

Project: 55041

Title: Molecular Characterization of a Novel Heavy Metal Uptake Transporter from Higher Plants & its Potential for use in Phytoremediation
PI: Dr. Julian I. Schroeder
Institution: University of California at San Diego



LCT1 Mediates Cadmium Uptake. Expression of the wheat gene, LCT1, in *S. cerevisiae* leads to dramatic hypersensitivity to cadmium, and increased intracellular accumulation. Clemens, S. *et. al* . (1998) *Proc. Natl. Acad. Sci. USA* **95**, 12043-12048. [see Project #55041]

Publication Type: Journal

Clemens, S., Kim, E. J., Neumann, D., & Schroeder, J. I. (1999). Tolerance to toxic metals by a gene family of phytochelatin synthases from plants and yeast. EMBO J. 18, 3325-3333.

Project: 55052

Title: Advanced Sensing and Control Techniques to Facilitate Semi-Autonomous Decommissioning

PI: Dr. Robert J. Schalkoff *Institution:* Clemson University

Publication Type: Journal

Costescu, N., Loffler, M., Zergeroglu, E., & Dawson, D. (1998, in press). Q robot - a multitasking PC based robot control system. Microcomputer Applications Journal Special Issue on Robotics.

Geist, R., Schalkoff, R., Stinson, T., & Gurbuz, S., (1997). Autonomous virtualization of real environments for telepresence applications. PRESENCE: Teleoperators and Virtual Environments, 6,6. MIT Press, 645 -657.

Publication Type: Proceeding

Costescu, N., Loffler, M., Zergeroglu, E., & Dawson, D. (1998, Sept.). Q robot: A Multitasking PC based robot control system. Proceedings of the IEEE Conference on Control Applications. Trieste, Italy. 892-896.

Geist, R., Vernon, D., & Schalkoff, R. (1998, Apr.). Rendering inversion in the automated construction of virtual environments. Proceedings of the 3rd ASCE Specialty Conf. on Robotics for Challenging Environments (ROBOTICS '98). Albuquerque, NM. 85 - 91.

Geist, R., Westall, J., Tregila, D., & Smotherman, M. (1998, Dec.). Real-time, 3-D graphics for the Linux PC. Proceeds of the 24th Annual Int. Conf. of the Computer Measurement Group (CMG98), Anaheim, CA. 863 - 873.

Van Pernis, A. (1999, Apr.). Surface construction from within a virtual environment. Proceedings of the Annual ACM Southeast Conference. Mobile, AL. NOTE: this was the winning paper in the ACM SE student paper competition.

Project: 55083

Title: Behavior of Dense, Immiscible Solvents in Fractured Clay-Rich Soils

PI: Dr. Larry D. McKay *Institution:* University of Tennessee at Knoxville

Publication Type: Journal

O-Hara, S. K., Parker, B. L., Jorgensen, P. R., & Cherry, J. A. (1999, in press). Trichloroethene DNAPL flow and mass distribution in naturally fractured clay. 1) Evidence of aperture variability. Water Resources Research.

Publication Type: Other

O'Hara, S. K. (1997). Solvent DNAPL flow and matrix diffusion in natural fractured clay: A large column experiment. MS thesis, Univ. of Waterloo. Ontario, Canada.

Publication Type: Paper

Cropper, S.C. (1998). Experimental observations of capillary pressure - saturation drainage of air and DNAPL in fractured shale saprolite. MS Thesis, Univ. of Tennessee. Knoxville, TN.

Publication Type: Presentation

Lenczewski, M., McKay, L. D., Sanseverino, J., & Knight, C. (1998, May 14-16). Sorption and microbiological factors controlling the fate and transport of TCE in fractured shale saprolite. Conference on Mass Transport in Fractured Aquifers and Aquitards, Univ. of Copenhagen, Denmark.

Lenczewski, M., McKay, L. D., Sanseverino, J., & Layton, A. (1999, Apr. 12-14). Biodegradation of TCE in fractured shale saprolite. Annual Meeting of the Tennessee Water Resources Association. Nashville, TN.

Lenczewski, M., McKay, L. D., Sanseverino, J., & Layton, A. (1999, May 30 - Jun. 3). Biodegradation of TCE in fractured weathered shale in east Tennessee. Annual Meeting of the American Society of Microbiology. Chicago, IL.

McKay, L., et al., (1998, Jul. 27-30). Behavior of dense, immiscible solvents in fractured clay-rich soils. Poster presented at DOE/EMSP Workshop. Chicago, IL.

McKay, L.D. (1998, May 14-16). Contaminant transport in highly weathered and fractured shales. Conference on Mass Transport in Fractured Aquifers and Aquitards. Univ. of Copenhagen, Denmark.

McKay, L.D. (1999, May 11-13). Field and laboratory studies of DNAPL behavior in fractured and highly weathered shale. University Consortium Solvents-in-Groundwater Workshop, Queen's University. Kingston, Ontario, Canada.

O'Hara, S. (1999, May 11-13). Characterizing solvent DNAPL migration pathways in fractured clay using a large column laboratory experiment. University Consortium Solvents-in-Groundwater Workshop, Queen's University. Kingston, Ontario, Canada.

O'Hara, S. K., Parker, B. L., Slough, K. J., & Sudicky, E. A. (1998, Dec.). Characterizing solvent DNAPL migration pathways in fractured clay using a numerical model and a large column laboratory experiment. American Geophysical Union (AGU) Fall Meeting, San Francisco, CA.

Parker, B. L., O'Hara, S. K., & Kirkpatrick, G. A. (1998, May 18-21). Solvent DNAPL flow in naturally fractured clay: Laboratory and field experiments. Presented at the First International Conference on Remediation of Chlorinated and Recalcitrant Compounds. Monterey, CA.

Parker, B.L. (1998, May 14-16). Diffusion profiles for identifying DNAPL migration pathways in a glaciolacustrine fractured clay. Conference on Mass Transport in Fractured Aquifers and Aquitards. Univ. of Copenhagen, Denmark.

Pitner, A., McKay, L. D., & Lenczewski, M. (1999, Apr. 12-14). DNAPL entry, dissolution, and diffusion in fractured shale saprolite. Annual Meeting of the Tennessee Water Resources Association. Nashville, TN.

Project: 55087

Title: Design and Synthesis of the Next Generation of Crown Ethers for Waste Separations: An Inter-Laboratory Comprehensive Proposal

PI: Dr. Bruce A. Moyer *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Moyer, B. A. (1999). Synergistic solvent extraction of Alkaline Earth Cations by Mixtures of Di-n-octylphosphoric Acid and Stereoisomers of Dicyclohexano-18-crown-6. Anal. Chem.,

Publication Type: Paper

Moyer, B. A. (1999, Mar 21-26). Calixarene Complexes with Alkali Cations: There is More to Binding Than You Realized. 217th American Chemical Society National Meeting, Anaheim, CA.

Moyer, B. A. (1999, Mar 21-26). Optimizing Cesium-Selective Extraction by Calix[4]arene Crown Ethers Through Ligand Design. 217th American Chemical Society National Meeting, Anaheim, CA.

Moyer, B. A. Probing the Source of Calixarens Selectivity: State-of-the-Art Quantum Calculations Reveal Multiple Binding Modes for Alkali Metals - Internal Report. Pacific Northwest National Laboratory.

Project: 55094

Title: Chemical and Ceramic Methods Toward Safe Storage of Actinides Using Monazite

PI: Dr. P. E. D. Morgan *Institution:* Rockwell International Corporation

Publication Type: Journal

Ewing, R. C., Lucas, G., Williams, J., & Zinkle, S. (Eds.). (1999). Radiation effects in nonmetals: Amorphization, phase decomposition, and nanoparticles. The Physical Review, 59,3981-92.

Meldrum, A., Boatner, L. A., & Zinkle, S. J. (no date given). A comparison of radiation effects in crystalline ABO sub-4-type phosphates and silicates. Minerological Magazine.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1998, in press). Effects of ionizing and displacive irradiation on several perovskite-structure oxides. Nuclear Instruments & Methods in Physics Research, Section B: Beam Interactions with Materials and Atoms v 141 n. Elsevier Sci B. V. 347-352, 0168-583X.

Meldrum, A., Boatner, L. A., & Zinkle, S. J. (1999, in press). Effects of dose rate and temperature on the crystalline-to-metamict transformation in the ABO sub-4 Orthosilicates. Canadian Mineralogist, 37,207-221.

Morgan, P. E. D. (1999). Radiation effects in nonmetals: Amorphization, phase decomposition, and nanoparticles. The Physical Review, 59, 3981-92.

Morgan, P. E. D. (1997). Lattice dynamics of xenotime: the phonon dispersion and density of states of LuPO4. The Physical Review, B56(11), 584.

Morgan, P. E. D. (no date given). Displacive radiation effects in the monazite and zircon structure orthophosphates. The Physical Review, B56.

Publication Type: Paper

Ewing, R. C., Lucas, G., Williams, J., & Zinkle, S. (Eds.). (1999, in press). The effect of temperature and damage energy on amorphization in zircon. MRS Proceedings Volume, Microstructural Processes in Irradiated Materials.

Ewing, R. C., Lucas, G., Williams, J., & Zinkle, S. (Eds.). (1999, in press). Radiation effects in zircon, hafnon, and thorite: Implications for Pu disposal. MRS Proceedings Volume, Microstructural Processes in Irradiated Materials.

Ewing, R. C., Lucas, G., Williams, J., & Zinkle, S. (Eds.). (1999, in press). Radiation effects in nonmetals: Amorphization, phase decomposition, and nanoparticles. MRS Proceedings Volume, Microstructural Processes in Irradiated Materials.

Meldrum, A., Boatner, L. A., & Ewing, R. C. (1999, Apr. 25-28). Radiation effects in Lanthanide-bearing AB04 compounds proposed for nuclear waste disposal. Presentation at the special focused session on Lanthanide-Containing Materials and Applications.

Morgan, P. E. D. (1999, Jun. 20-23). Magnetic and thermodynamic properties of rare-earth orthophosphates and pentaphosphates. 15th University Conference on Glass Science.

Project: 55100

Title: Human Genetic Marker for Resistance to Radiations and Chemicals
PI: Dr. Howard B. Lieberman *Institution:* Columbia University

Publication Type: Journal

Hang, H., Rauth, S. J., Hopkins, K. M., Davey, S. K., & Lieberman, H. B. (1998). Molecular cloning and tissue-specific expression of Mrad9, a murine orthologue of the Schizosaccharomyces pombe rad9+ checkpoing control gene. J. Cell Physiol., 177,232-240.

Project: 55103

Title: Utilization of Kinetic Isotope Effects for the Concentration of Tritium
PI: Dr. Gilbert M. Brown *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Huynh, M. H. V., et. al. (1999). Oxo-like reactivity of high oxidation state osmium hydrazido complexes. Journal of American Chemical Society, 121,1403-1404.

Huynh, M. H. V., White, P. S., & Meyer, T. J. (1999, in press). Proton-coupled electron transfer from nitrogen: A N-H/N-D Kinetic Isotope Effect of 41.4". Journal of American Chemical Society.

Lebeau, E. L. & Meyer, T.J. (1999). Oxidation of benzyl alcohol by a dioxo complex of Ru(VI). Inorganic Chemistry, 38,2174-2181.

Trammell, S. A., et. al. (1998). Mechanisms of surface electron transfer: Proton-coupled electron transfer. Journal of American Chemical Society, 120,13248-13249.

Project: 55108

Title: Monitoring Genetic & Metabolic Potential for In Situ Bioremediation: Mass Spectrometry
PI: Dr. Michelle V. Buchanan *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Hurst, G. B., et. al. (1998). MALDI-TOF analysis of polymerase chain reaction products from methanotrophic bacteria. Analytical Chemistry, 70,2693-2698.

Publication Type: Paper

Kim, Y., Hurst, G., Doktycz, M., & Buchanan, M. (1999, Jun. 13-18). Improved spot homogeneity for DNA MALDI matrices. Presentation at the 47th ASMS conference on Mass Spectrometry and Allied Topics. Dallas, TX.

Publication Type: Poster

Buchanan, M. V. (1997, Nov. 9). Improved mass spectrometric resolution for PCR product size measurement. DOE Human Genome Program Contractor-Grantee Workshop VI, Santa Fe, NM.

Buchanan, M. V. (1998, Jan. 24). TOF-MS detection of PCR products. 10th Sanibel Conference on Mass Spectrometry, Sanibel Island, FL.

Buchanan, M. V., et. al. (1998, Jul. 27-30). Monitoring genetic and metabolic potential for in situ bioremediation: Mass spectrometry. Poster presentation at the DOE Environmental Management Science Program Workshop, Chicago, IL.

Hurst, G. B., Kim, Y., Weaver, K., & Buchanan, M. V. (1999, Jan. 12-16). PCR product size measurement using MALDI mass spectrometry. Poster presentation at the 7th DOE Human Genome Contractor-Grantee Workshop. Oakland, CA.

Publication Type: Presentation

Hurst, G. B., Weaver, K., & Buchanan, M. V. (1997, Nov. 9-13). Improved mass spectrometric resolution for PCR product size measurement. Presentation at the Sixth Department of Energy Contractor and Grantee Workshop of the Human Genome Program, Santa Fe, NM.

Kim, Y., Hurst, G. B., Doktycz, M. J., & Buchanan, M. V. (1999, Jun. 13-18). Improved spot homogeneity for DNA MALDI matrices. Presentation at the 47th ASMS Conference on Mass Spectrometry and Allied Topics. Dallas TX.

Publication Type: Proceeding

Hurst, G. B., et. al. (1998, May 31 - Jun. 4). Identification of methanotrophic bacteria using the polymerase chain reaction with MALDI-TOF detection. Proceedings of the 46th ASMS Conference on Mass Spectrometry and Allied Topics. Orlando FL. 1202.

Hurst, G. B., Weaver, K., Buchanan, M. V., & Doktycz, M. J. (1997, Jun. 1-5). Analysis of PCR products using delayed-extraction MALDI-TOF. Proceedings of the 45th ASMS Conference on Mass Spectrometry and Allied Topics. Palm Springs CA. 843.

Weaver, K., Doktycz, M. J., Britt, P. F., Hurst, G. B., & Buchanan, M. V. (1998, May 31 - Jun. 4). 96-well microtiter-format purification of DNA for MALDI-TOF analysis. Proceedings of the 46th ASMS Conference on Mass Spectrometry and Allied Topics. Orlando FL. 60.

Project: 55110

Title: An Alternative Host Matrix Based on Iron Phosphate Glasses for the Vitrification of Specialized Nuclear Waste Forms

PI: Dr. Delbert E. Day *Institution:* University of Missouri-Rolla

Publication Type: Journal

Day, D. E. (1997). Structural features of iron-phosphate glasses. J. Non-Cryst. Solids, 222,144.

Day, D. E. (1997). Structural study of iron phosphate glasses. Phys. Chem. Glasses, 38,74.

Day, D. E. (1998). Chemically durable iron phophate glass wasteforms. J. Non-Cryst. Solids, 241,1.

Day, D. E. (1998). On the structure and radiation chemistry of iron phosphate glasses: New insights from electron spin resonance and evolved gas mass spectroscopy. Nucl. Inst. Meth. Phys. Res. B, 141,600.

Day, D. E. (1998). Redox characteristics and structural properties of iron phosphate glasses: A potential host matrix for vitrifying high level nuclear waste. Ceramic Transactions, 87,261.

Publication Type: Proceeding

Day, D. E. (1999). Effects of nuclear waste components on redox equilibria, structural features, and crystallization characteristics of iron phosphate glasses. Environment Issues and Waste Management Technologies IV: Ceramic Transactions, 93,195.

Day, D. E. (1999). Iron redox equilibria and crystallization of iron phosphate glasses. Environment Issues and Waste Management Technologies IV: Ceramic Transactions, 93,187.

Project: 55118

Title: Plant Rhizosphere Effects on Metal Mobilization and Transport

PI: Dr. Teresa W. M. Fan *Institution:* University of California at Davis

Publication Type: Journal

Fan, T. W. -M., Pedler, J., Lane, A. N., Crowley, D., & Higashi, R. M. (1997). Comprehensive analysis of organic ligands in whole root exudates using NMR and GC-MS. Analytical Biochemistry, 251,57-68.

Higashi, R. M., Fan, T. W. -M., & Lan, A. N. (1998). Association of desferrioxamine with humic substances and their interaction with cadmium(II) as studied by pyrolysis gas chromatography mass spectrometry and nuclear magnetic resonance spectroscopy. Analyst, 123(5),911-918.

Publication Type: Other

Fan, T. W. -M. & Lane, A. N. (1999, in press). NMR in the plant-soil environment. In Encyclopedia of NMR Spectroscopy, John Wiley and Sons, New York, NY.

Fan, T. W. -M. (1996). Recent advancement in profiling plant metabolites by multi-nuclear and multi-dimensional NMR. In Shachar-Hill, Y., & Pfeffer, P. E. (Eds.), Nuclear Magnetic Resonance in Plant Biology. American Society of Plant Physiologists. Rockville, MD. 181-254.

Publication Type: Presentation

Fan, T. W. -M., Higashi, R. M., & Crowley, D. E. (1998, Jul.). Plant rhizosphere effects on metal mobilization and transport. DOE EMSP Symposium, Chicago, IL.

Fan, T. W. -M., Shenker, M., Higashi, R. M., Crowley, D. E., & Lane, A. N. (1999, Mar.). Rhizosphere mobilization of heavy metals via plant root exudation. Semi-Annual Meeting of American Chemical Society, Anaheim, CA.

Fan, T. W. -M., Shenker, M., Lane, A. N., Crowley, D., & Higashi, R. M. (1998, Apr.). Comprehensive determination of root exudates under combined Fe deficiency/CD stress by NMR and GC-MS. Society of Environmental Toxicology and Chemistry-Europe. Bordeaux, France.

Higashi, R. M. & Fan, T. W. -M. (1998, May). Ternary interactions of Cd(II), ligands, and humic substances - implications for metal ion bioavailability. EPA, DOE, ONR, & NSF Joint Workshop.

Higashi, R., Fan, T., Baraud, F., & Lane, A. (1999, Mar.). Ternary interactions of biogenic ligands and Cd(II) with humic substances, with implications for metal ion bioavailability. Semi-annual meeting of the American Chemical Society, Anaheim, CA.

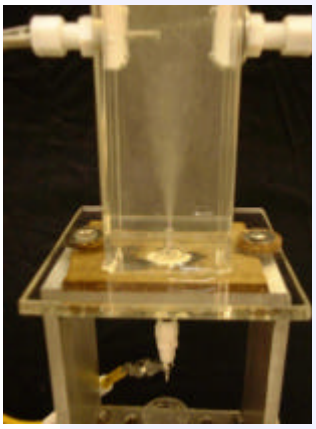
Project: 55119

Title: Phase Equilibria Modification by Electric Fields
PI: Dr. Costas Tsouris *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Blankenship, K. D., DePaoli, D. W., Hylton, J. O., & Tsouris, C., (1999). Effect of electrode configurations on phase equilibria with electric fields. Separation and Purification Technology, 15,283-294.

Blankenship, K. D., DePaoli, D. W., Hylton, J. O., & Tsouris, C. (1999). Effect of electrode configurations on phase equilibria with electric fields. Separation and Purification Technology, 15,283-294.



Simultaneous pumping, spraying, and mixing of a gas in an aqueous solution by means of an electric field can be used for the removal of contaminants from the solution. [see Project #55119]

Blankenship, K. D., Shah, V. M., & Tsouris, C. (1999). Distillation under electric fields. Separation Science and Technology.

Blankenship, K. D., Shah, V. M., & Tsouris, C. (1999, in press). Distillation under electric fields. Separation Science and Technology, 34,1393-1409.

Norato, M. A., Tsouris, C., & Tavlarides, L. L. (1998). Phase inversion studies in liquid-liquid dispersions. The Canadian Journal of Chemical Engineers, 76,486-494.

Shin, W-. T., Yiacoumi, S., & Tsouris, C. (1997). Experiments on electrostatic dispersion of air in water. Industrial and Engineering Chemistry Research, 36,3647-3655.

Tsouris, C. W., Shin, T., Yiacoumi, S., & DePaoli, D. W. (1999, in press) Effects of electric fields on bubble and particle velocities in water and alcohols. Journal of Colloid and Interface Science.

Tsouris, C., Borole, A. A., Kaufman, E. N., & DePaoli, D. W. (1999, in press). An electrically driven gas-liquid-liquid contractor for bioreactor and other applications. Industrial and Engineering Chemistry Research, 38,1877-1883.

Tsouris, C., Borole, A. P., & Kaufman, E. N., DePaoli, D. W. (1999). An electrically driven gas-liquid-liquid contactor for bioreactor and other applications. Industrial and Engineering Chemistry Research, 38, 1877-1883.

Tsouris, C., Borole, A. P., Kaufman, E. N., & DePaoli, D. W. (1999, in press) An electrically driven gas-liquid-liquid contactor for bioreactor and other applications. Industrial and Engineering Chemistry Research.

Tsouris, C., DePaoli, D. W., & Yiacoumi, S., (1999, Jun. 1). Novel environmental technologies driven by electric and magnetic fields. Environmental Technologies and Opportunities Forum. Oak Ridge, TN.

Tsouris, C., Shin, W.- T. & Yiacoumi, S. (1998). Pumping, spraying, and mixing of fluids by electric fields. The Canadian Journal of Chemical Engineers, 76,589-599.

Publication Type: Other

Blankenship, K. D. (1999, Mar.). Distillation under electric fields. Master Thesis, Department of Chemical Engineering, University of Tennessee. Knoxville, TN.

Publication Type: Paper

Blankenship, K. D. (1999, Apr.). Distillation with applied electric fields. Master Thesis, Department of Chemical Engineering, University of Tennessee. Knoxville, TN.

Tsouris, C., & Dong, J. (1999, Jun. 13-16). Electric-effects on fluid interfaces. 73rd ACS Colloid and Surface Science Symposium, Massachusetts, Institute of Technology. Cambridge, MA.

Project: 55179

Title: Acoustic Probe for Solid-Gas-Liquid Suspensions
PI: Dr. Lawrence L. Tavlarides *Institution:* Syracuse University

Publication Type: Journal

Spelt, P. D. M., Norato, M. A., Sangani, A. S., & Tavlarides, L. L. (1999). Determination of particle size distributions from acoustic wave propagation measurements. Phys. Fluids, 11,1065-1080.

Project: 55188

Title: Chemical Decomposition of High-Level Nuclear Waste Storage/Disposal Glasses Under Irradiation
PI: Dr. David L. Griscom *Institution:* Naval Research Laboratory

Publication Type: Journal

Griscom, D. L., Merzbacher, C. I., Weeks, R. A., & Zuhr, R. A. (1999). Electron spin resonance studies of defect centers induced in a high-level nuclear waste glass simulant by gamma-irradiation and ion-implantion. J. Non-Cryst. Solids 258,34-47.

Project: 55196

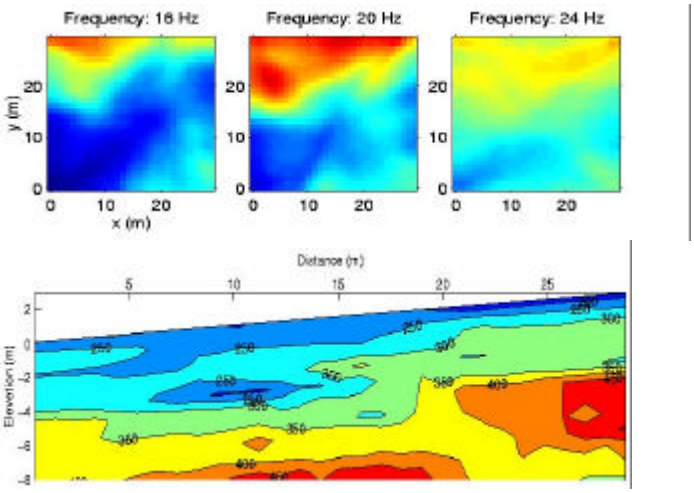
Title: In Situ, Field Scale Evaluation of Surfactant Enhanced DNAPL Recovery Using a Single-Well, Push-Pull Test
PI: Dr. Jonathan D. Istok *Institution:* Oregon State University

Publication Type: Journal

Field, J. A., Istok, J. D., Schroth, M. H., Sawyer, T. E., & Humphrey, M. D. (1999, in press). Laboratory investigation of surfactant-enhanced TCE solubilization using single-well, 'push-pull' tests. Ground Water.

Field, J.A., & Istok, J. D. (1999). Comment on estimation of nonaqueous phase liquid-water interfacial areas in porous media following mobilization by chemical flooding. Environmental Science and Technology, 32(2),3836-3837.

Istok, J. D., Field, J. A., Schroth, M. H., Sawyer, T. E., & Humphrey, M. D. (1999). Laboratory and field investigation of surfactant sorption ssing single-well 'push-pull' tests. Ground Water.



Ever wonder what is under here? Generate a set of Group Velocity images (upper right), then invert the dispersion curves at each position to get an image of the shear-wave structure (lower right). The low velocity at 10m and 4m depth is a suspected burial trench, or the high uplifted under 25m could indicate a thrust fault. [see Project #55218]

Project: 55218

Title: Seismic Surface-Wave Tomography of Waste Sites
PI: Dr. Timothy L. Long *Institution:* Georgia Institute of Technology

Publication Type: Other

Long, L. T. (1999, Feb.). Seismic surface wave tomography at waste sites. Research Note in Fast Times, the EEGS Newsletter.

Publication Type: Paper

Long, L. T. & Kocaoglu, A. (1999, Oct. 16-20). A tomographic inversion method for near-surface structure. Eastern Section Seismological Society of America Annual Meeting. Memphis, TN.

Long, L. T., Kocaoglu, A., Doll, W. E., Chen, X. Q., & Martin, J. (1999, Oct.). Surface-wave group-velocity tomography for shallow structures at a waste site. SEG Expanded Abstract, Annual Meeting. Houston, TX.

Publication Type: Proceeding

Long, L. T., & Kocaoglu, A. (1999, Mar.). Surface-wave group-velocity tomography for shallow structures. Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems, Environmental and Engineering Geophysical Society (SAGEEP99).

Project: 55267

Title: Containment of Toxic Metals and Radionuclides in Porous and Fractured Meda: Optimizing Biogeochemical Reduction Versus Geochemical Oxidation
PI: Dr. Philip M. Jardine *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Barnett, M. O., Jardine, P. M., Brooks, S. C., & Selim, H. M. (1999, in press). Adsorption and transport of U(VI) in subsurface media. Soil Sci. Soc. Am. J.

Brooks, S. C., & Barnett, M. O. (1999). Uranium sorption to bacterial cells as a related to metal reduction capabilities in the presence of porous media. Appl. and Eniron. Micro.

Brooks, S. C., Carroll, S. L., & Jardine, P. M. (1999, in press). Sustained bacterial reduction of Co(III)EDTA in the presence of competing geochemical oxidation during dynamic flow. Environ. Sci. Technol.

Fendorf, S. E., Jardine, P. M., Patterson, R. R., Taylor, D. L., & Brooks, S. C. (1999, in press). Pyrolusite surface transformations measured in real-time during the reactive transport of Co(II)EDTA. Geochim. Cosmochim. Acta.

Jardine, P. M., et. al. (1999, in press). Quantifying diffusive mass transfer in fractured shale bedrock. Water Resour. Res.

Jardine, P. M., et. al. (1999,in press). Fate and transport of hexavalent chromium in undisturbed heterogeneous soil. Environ. Sci. Technol.

Publication Type: Other

Jardine, P. M., Brooks, S. C., Wilson, G. V., & Sanford, W. E. (1999, in press). Basic research strategies for resolving remediation needs in contaminated fractured subsurface media. In Faybishenko, B. (Ed.), Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. American Geophysical Union, Geophysical Monograph Series.

Jardine, P. M., O'Brien, R., Wilson, G. V., & Gwo, J. P. (1998). Experimental techniques for confirming and quantifying physical nonequilibrium processes in soils. In Selim, H. M. & Ma, L. (Eds.), Physical Nonequilibrium in Soils: Modeling and Application. Ann Arbor Press, Inc. Chelsea, MI. 243-271.

Jardine, P. M., Wilson, G. V., Luxmoore, R. J., & Gwo, J. P. (1999, in press). Conceptual Model of Vadose-Zone Transport in Fractured Weathered Shales. In Hsieh, P. A. (Ed.), Conceptual Models of Flow and Transport in the Fractured Vadose Zone. National Research Council.

Publication Type: Presentation

Brooks, S. C., & Jardine, P. M. (1997, Oct. 26-31). Bacterial reduction of toxic metals during dynamic flow. American Society of Agronomy. Anaheim, CA.

Fendorf, S., Jardine, P. M., & Brooks, S. C. (1997, Apr. 13-17). Sorption induced inhibition of redox reactions involving manganese oxides. American Chemical Society. San Francisco, CA.

Guha, H., Saiers, J. E., Jardine, P. M., & Brooks, S. C. (1998, Dec. 6-10). Development and evaluation of a mathematical model for oxidation, sorption, and transport of Co(II)EDTA 2-. American Geophysical Union. San Francisco, CA.

Jardine, P. M. (1997, Apr. 13). Sorption induced inhibition of redox reaction involving manganese oxides. American Chemical Society. San Francisco, CA.

Jardine, P. M. (1997, Oct. 12). Geochemical processes governing the fate and transport of Cr(III) and Cr(VI) in soils. Soil Science Society of America. Anaheim, CA.

Jardine, P. M. (1997, Oct. 26). Bacterial reduction of toxic metals during dynamic flow. Science Society of America. Anaheim, CA.

Jardine, P. M., et. al. (1999, Feb. 6-10). Basic research strategiesn for resolving remediation needs in contaminated fractured subsurface media. Symposium on Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. Lawrence Berkeley National Laboratory. Berkeley, CA.

Jardine, P. M., Wilson, G. V., Sanford, W. E., & Luxmoore, R. J. (1998, May 14-16). Exploring subsurface transport mechanisms in fractured media at laboratory and field scales. Conference on “Mass transport in fractured aquifers and aquitards” Geological Institute, Unversity of Copenhagen, Denmark.

Mayes, M. A., Reedy, O. C., Larsen, I. L., Brooks, S. C., & Jardine, P. M. (1997, Oct.). Multispecies contaminant transport in undisturbed columns of weathered fractured shale. Geologic Society of America.

Mayes, M. A., Reedy, O. C., Larsen, I. L., Brooks, S. C., & Jardine, P. M. (1997,Oct. 26-31). Multispecies contaminant transport in undisturbed columns of weathered fractured shale. American Society of Agronomy. Anaheim, CA.

Mehlhorn, T. L., Jardine, P. M., Brooks, S. C., Fendorf, S. E., & Saiers, J. E. (1997, Oct. 26-31). Geochemical processes governing the fate and transport of Cr(III) and Cr(VI) in soils. American Society of Agronomy. Anaheim, CA.

Sanford, W. E., & Jardine, P. M. (1997, Oct. 26-31). Examining diffusion with multiple tracers to aid remediation of contaminated sites. American Society of Agronomy. Anaheim, CA.

Zhang, C., Brooks, S., Fendorf, S., & Jardine, P. (1998, Aug.). Microbial uranium reduction and biomineralization: implication for immobilization of toxic metals and radionuclides. 17th Annual Meeting of the International Mineralogical Association, Toronto, Canada.

Publication Type: Press release

Evans, R. & Hill, D. (1999). Press release initated by Department of Energy. One of 5 out of 200 EMSP projects to be featured in a press release package.

Norton, D. (1999, summer). Press release intiated by waste policy institute of Blacksburg, VA.

Publication Type: Proceeding

Fendorf, S. E., Jardine, P. M., Taylor, D. L., & Brooks, S.C. (1999). Auto-inhibition of oxide mineral oxidative capacity toward Co(II)EDTA: Time-resolved studies using XANES spectroscopy. In Sparks, D. L. & Grundel, T. (Eds.), Kinetics and mechanisms of sorption processes at the mineral-water interface. ACS Symposium Series 715,358-371.

Jardine, P. M. (1998, Aug. 24-28). Can basic research on contaminant transport be used to improve the design of remedial strategies? Proceedings of "School of Environmental Science and Technology". Buenos Aires, Argentina.

Jardine, P. M. (1998, Dec. 31). Auto-inhibition of oxide mineral oxidation capacity toward Co(II) EDTA: Time-resolved studies using XANES spectroscopy. In Sparks, D. L., & Grundel, T. (Eds.), Kinetics and mechanisms of sorption processes at the mineral-water interface. ACS Symposium Series.

Project: 55276

Title: Fundamental Chemistry and Thermodynamics of Hydrothermal Oxidation Processes

PI: Dr. John M. Simonson *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Blencoe, J. G., Anovitz, L. M., & Seitz, J. C. (1998, in press). A new method for modeling the thermodynamic mixing properties of high-temperature H2 O-CO2 fluids. Eos,79.

Blencoe, J. G., Seitz, J. C., & Anovitz, L. M., (1999, in press). The CO2 -H2 O System. II. Calculated Thermodynamic Mixing Properties for 400°C, 0-400 MPa. Geochim. Cosmochim. Acta, 63.

Chialvo, A. A., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (1999). Solvation in high-temperature electrolyte solutions. I. Hydration shell behavior from molecular simulation. J. Chem. Phys. 110,1064-1074.

Chialvo, A. A., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (1999). Solvation in high-temperature electrolyte solutions. II. Some formal results. J. Chem. Phys. 110,1075-1086.

Chialvo, A. A., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (1998). Thermodynamics and kinetics of ion speciation in supercritical aqueous solutions: A molecular-based study. Fluid Phase Equilibria 150-151,107-115.

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Moore, R. C., Mesmer, R. E., & Simonson, J. M. (1997). The solubility of potassium carbonate in water between 384 and 529 K measured using the synthetic method. J. Chem. Eng. Data 42,1078-1081.

Seitz, J. C. & Blencoe, J. G. (1999, in press). The CO2 -H2 O System. I. Experimental Determination of Volumetric Properties at 400°C, 10-100 MPa. Geochim. Cosmochim. Acta, 63.

Publication Type: Presentation

Blencoe, J. G., Anovitz, L. M. & Seitz, J. C. (1998). A Helmholz free energy model for supercritical H2 O-CO2 mixtures. Geol. Soc. Amer. Abs. with Prog., 30,A-319.

Blencoe, J. G., Anovitz, L. M., Seitz, J. C. (1997). Serious shortcomings of semi-empirical equations of state for high-temperature aqueous C-O-H-N fluids. Geol. Soc. Amer. Abs. with Prog. 29,A-210.

Seitz, J. C. & Blencoe, J. G. (1997). Experimentally determined volumetric properties and solvus relations for H2 O-CO2 -N2 mixtures at 300°C and pressures < 1000 bars. Geol. Soc. Amer. Abs. with Prog. 29,A-209.

Singh, J., Blencoe, J. G., & Seitz, J. C., (1998). Experimentally determined excess molar volumes for H2 O-N2 fluids at 300°C, 75-1000 bars. Geol. Soc. Amer. Abs. with Prog., 30,A-319.

Project: 55278

Title: Molecular Genetics of Metal Detoxification: Prospects for Phytoremediation
PI: Dr. David W. Ow *Institution:* U.S. Dept. of Agriculture

Publication Type: Journal

VandeWeghe, J. & Ow, D. W. (1999). A fission yeast gene for mitochondrial sulfide oxidation. Journal of Biological Chemistry, 274,13250-13257.

Ow, D. W. (1996). Heavy metal tolerance genes: Prospective tools for bioremediation. Resources, Conservation, and Recycle 18,135-149.

Perego, P., VandeWeghe, J., Ow, D. W., & Howell, S. B. (1997). The role of determinants of cadmium sensitivity in the tolerance of Schizosaccharomyces pombe to cisplatin. Molecular Pharmacology 51,12-18.

Publication Type: Other

Ow, D. W. (1998). Prospects of engineering heavy metal detoxification genes in plants. In Shewry, P. (Ed.), Engineering Crops for Industrial Uses. Portland Press. 111-124.

Publication Type: Presentation

Ow, D. W. (1996, Sept. 16-18). Prospects of engineering heavy metal detoxification genes in plants. Abstracts of the Symposium on Engineering Crops for Industrial End Uses. Bristol, England.

Ow, D. W. (1997, Sept. 29 - Oct. 1). Heavy metal tolerance genes as tools for phytoremediation. Abstracts of the International Symposium on Environmental Engineering. Kyongju, Korea.

Ow, D. W., Clark, S., Henstrand, J., & Kim, J. (1998, Jun. 19-20). Molecular genetics of heavy metal tolerance. Abstracts of the University of Connecticut Agricultural Biotechnology Symposium, Storrs, CN.

Ow, D. W., et. al. (1997, Sept. 21-27). Heavy metal tolerance genes for phytoremediation. Abtracts of the 5th International Congress of Plant Molecular Biology, Singapore.

Ow, D. W., et. al. (1998, Jul. 27-30). Heavy metal tolerance genes. Abstracts of the DOE Environmental Remediation Meeting. Chicago, IL.

VandeWeghe, J. & Ow, D. W. (1996, Aug. 6-11). An oxidoreductase-like gene required for cadmium tolerance in Schizosaccharomyces pombe. Abstracts of the 1996 Yeast Genetics & Molecular Biology Meeting. Univ. of Wisconsin. Madison, WI. 309.

VandeWeghe, J., Ow, D. W. (1997, Apr. 7-8). A novel mitochrondrial oxidoreductase required for phytochelatin accumulation and cadmium tolerance in fission yeast. Abstracts of the Society for Experimental Biology Annual Meeting, Session on Metals and Genes. Canterbury, England. 80.

Zankel, T. C. & Ow, D. (1996, Mar. 17-23). Homologs of the human BTF3 and Wiskott-Aldrich syndrome proteins are involved in the metal stress response of S. pombe. Abstracts of the 1996 Keystone Symposium on Transcriptional Mechanisms. Taos, NM. 67.

Zankel, T. C., Ow, D. W. (1997, Mar. 31 - Apr. 6). A Schizosaccharomyces pombe homolog of the Wiskott-Aldrich syndrome protein is involved in stress adaptation and mating. Abstracts of the 1997 Keystone Symposium on Temporal and Spatial Determinants of Specificity in Signal Transduction, Keystone, CO.

Publication Type: Proceeding

Perego, P, Vandeweghe, J, Ow, D, & Howell, S B. (1997). Role of determinants of cadmium sensitivity in the sensitivity of Schizosaccharomyces pombe to cisplatin. Eighty-eighth Annual Meeting of the American Association for Cancer Research, San Diego, CA. Also in the proceedings of the American Association for Cancer Research Annual Meeting, 38,393.

Perego, P., VandeWeghe, J., Ow, D., & Howell, S. B. (1996, Apr. 20-24). Mechanisms of resistance to cisplatin (DDP) in Schizosaccharomyces pombe. 87th Annual Meeting of the American Association for Cancer Research. Washington, D. C. Proceedings of the American Association for Cancer Research Annual Meeting, 37,336.

Project: 55294

Title: Superconducting Open-Gradient Magnetic Separation for the Pretreatment of Radioactive or Mixed Waste Vitrification Feeds

PI: Richard D. Doctor *Institution:* Argonne National Laboratory

Publication Type: Paper

Doctor, R. D. (1997, Oct. 24). Superconducting open-gradient magnetic separation for the pre-treatment of radioactive or mixed-waste vitrification feeds. Tenth Symposium on Separation Science and Technology for Energy Applications.

Project: 55318

Title: Improved Analytical Characterization of Solid Waste Forms by Fundamental Development of Laser Ablation Technology

PI: Dr. Richard E. Russo *Institution:* Lawrence Berkeley National Laboratory

Publication Type: Journal

Borisov, O. V., Mao, X. L., & Russo, R. E. (1999, in press). Laser ablation ICP/MS calibration based on binary Cu/Zn alloy standards. Spectrochimica Acta B.

Borisov, O. V., Mao, X. L., Ciocan, A. C., & Russo, R. E. (1998). Time resolved parametric studies of laser ablation using ICP-AES. Applied Surface Science 129,315.

Chan, W. T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1998). Effects of gas environment on pico-second laser ablation. Applied Surface Science 129,269.

Ciocan, A. C., Mao, X. L., Borisov, O. V., & Russo, R. E. (1998). Optical emission spectroscopy of the influence of laser ablated mass on dry inductively coupled plasma conditions. Spectrochimica Acta, 53B,463.

Leung, A. P. K., Chan, W. T., Mao, X. L., & Russo, R. E. (1998). Influence of gas atmosphere on picosecond laser ablation sampling efficiency and ICP-AES. Analytical Chemistry, 70(N22),4709.

Russo, R. E. (1998). Laser ablation sampling. Trends in Analytical Chemistry (Personal Edition), 17(8-9).

Russo, R. E. (1998, Jul. 1). Transient isotachophoretic - electrophoretic separations of lanthanides with indirect laser-induced fluorescence detection. Analytical Chemistry, 70(13).

Russo, R. E. (1998, Jul. 18). Preferential vaporization during laser ablation inductively coupled plasma atomic emission spectroscopy. Applied Spectroscopy, 52(7).

Russo, R. E. (1998, Mar. 30). Optical emission spectroscopy studies of the influence of laser ablated mass on dry inductively coupled plasma conditions. Spectrochimica Acta, Part B: Atomic Spectroscopy, 53(3).

Russo, R. E. (1998, May 29). Enhancements in laser ablation inductively coupled plasma-atomic emission spectrometry based on laser properties and ambient environment. Spectrochimica Acta, Part B: Atomic Spectroscopy, 53(5).

Russo, R. E. (1998, Nov. 15). Influence of gas environment on picosecond laser ablation sampling efficiency and ICP conditions. Analytical Chemistry, 70(22), Washington, D. C., 4709-4716.

Publication Type: Presentation

Borisov, O. V., Mao, X. L., & Russo, R. E. (1998, Oct.). Optimization of ICPMS for laser ablation sampling. 25th Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Austin, TX.

Chan, W. -T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1997, Oct.). Effect of gas medium on laser ablation sampling for ICP-AES. Twenty-Fourth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies. (FACSS). Providence, RI.

Chan, W. T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1997, Jul.). Effects of gas atmosphere on pico-second laser ablation sampling for ICP-AES. Fourth International Conference on Laser Ablation (COLA 97). Asilomar, CA.

Ciocan, A. C., Mao, X. L., Borisov, O. V., & Russo, R. E. (1997, Jul.). Optical emission spectroscopy of the influence of ablated material on dry inductively coupled plasma conditions. COLA 97. Asilomar, CA.

Russo, R. E. (1998, Sept.). Laser-ablation sampling with ICP/AES and ICP/MS: Fundamental issues to improve analytical applications. Invited presentation at the Society of Applied Spectroscopy California Section Meeting. Fremont, CA.

Russo, R. E. (1999, Apr.). Fundamental and applied aspects of laser ablation for chemical analysis. Frontiers in Chemistry Lecture Series. Wayne State University. Detroit, MI.

Russo, R. E., Jeong, S. H., Mao, X. L., Borisov, O. V., & Yoo, J. (1998, Oct.). Particle generation and transport during laser ablation sampling for chemical analysis. 25th Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Austin, TX.

Russo, R. E., Mao, X. L., Ciocan, A. C., & Borisov, B. V. (1997, Oct.). Laser ablation solid sample chemical analysis: Dream or reality. Invited presentation at the Twenty-Fourth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Providence, RI.

Russo, R. E., Mao, X. L., Ciocan, A. C., & Borisov, B. V. (1997, Oct.). Laser ablated mass influence on the properties of the ICP. Invited presentation at the Twenty-Fourth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies. (FACSS). Providence, RI.

Publication Type: Proceeding

Borisov, O. V., Mao, X. L. & Russo, R. E. (1999, Apr.). Direct characterization of solid waste forms using laser ablation ICPMS. Waste Management Science and Technology in the Ceramic and Nuclear Industries. American Ceramic Society.

Chan, W. T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1997). Effects of gas atmosphere on pico-second laser ablation sampling for ICP-AES. Fourth International Conference on Laser Ablation (COLA 97). Asilomar, CA.

Ciocan, A. C., Mao, X. L., Borisov, O. V., & Russo, R. E. (1997, Jul.). Optical emission spectroscopy studies of ablated material on dry inductively coupled plasma conditions. COLA. Asilomar, CA.

Mao, X. L., Ciocan, A. C., Borisov, O. V., & Russo, R. E. (1997, Jul.). Time resolved parametric studies of laser ablation of brass using ICP-AES. COLA 97. Asilomar, CA.

Mao, X. L., Ciocan, A. C., Borisov, O. V., & Russo, R. E. (1997, Jul.). Time resolved parametric studies of laser ablation of brass using ICP-AES. COLA. Asilomar, CA.

Russo, R. E. (1997, Jul. 21-25). Effects of gas environment on picosecond laser ablation. Applied Surface Science Proceedings of the 1997 4th International Conference on Laser Ablation, 127-129.

Russo, R. E. (1997, Jul. 21-25). Propagation of the shock wave generated from excimer laser heating of aluminum targets in comparison with ideal blast wave theory. Applied Surface Science Proceedings of the 1997 4th International Conference on Laser Ablation, 127-129.

Russo, R. E. (1997, Jul. 21-25). Time-resolved parametric studies of laser ablation using inductively coupled plasma atomic emission sectroscopy. Applied Surface Science Proceedings of the 1997 4th International Conference on Laser Ablation, 127-129.

Russo, R. E., Mao, X. L., & Borisov, O. V. (1998). Laser Ablation Sampling. Trends in Analytical Chemistry,17,461.

Project: 55328

Title: Novel Analytical Techniques Based on an Enhanced Electron Attachment Process

PI: Dr. Lal A. (TENN) *Institution:* University of Tennessee at Knoxville

Publication Type: Journal

Ding, W., McCorkle, D. L., & Pinnaduwage, L. A. (1998). Enhanced formation of negative ions by electron attachment to highly-excited molecules in a flowing afterglow plasma. J. Appl. Phys. 84,3051.

Ding, W., Pinnaduwage, L. A., Tav, C., & McCorkle, D. L. (1999, in press). The role of high Rydberg states in enhanced O-formation in a pulsed O2 discharge. Plasma Sources Sci. Technol., 8,384.

Nagesha, K. & Pinnaduwage, L. A. (1998). O-formation from O2 via Rydberg-Rydberg electron transfer. J. Chem. Phys. 109,7124.

Pinnaduwage, L. A. & Zhu, Y. (1997). Long-time stability of superexcited high-Rydberg molecular states. Chem. Phys. Lett., 277,147.

Pinnaduwage, L. A. & Zhu, Y. (1998). High-Rydberg fragment formation via core dissociation of superexcited Rydberg molecules. J. Chem. Phys. 108, 6633.

Pinnaduwage, L. A., et. al. (1999). Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges. J. Appl. Phys., 85,7064.

Pinnaduwage, L. A., McCorkle, D. L., & Ding, W. (1997). Enhanced electron attachment to highly excited molecules using a plasma mixing scheme. Appl. Phys. Lett. 71,3634.

Pinnaduwage, L. A., Nagesha, K., Zhu, Y., Buchanan, M. V., & Hurst, G. B. (1999, in press). Laser-enhanced negative ion mass spectroscopy for weakly-electron-ataching species. Int. J. Mass Spectrom, Ion Processes.

Publication Type: Presentation

Nagesha, K. & Pinnaduwage, L. A. (1999, Oct. 5-8). Magnetic and electric field induced enhancements in laser induced anion formation. 52nd Annual Gaseous Electronics Conference. Norfolk, Virginia.

Pinnaduwage, L. A., Buchanan, M. V., & Hurst, G. B. (1998, Jul. 27-30). Novel analytical techniques based on an enhanced electron atachment process. Presented at the Environmental Management Science Program Workshop, Chicago, IL.

Pinnaduwage, L. A., Ding, W. & McCorkle, D. L. (1999, Oct. 5-8). Negative ion formation in pulsed plasmas. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Tav, C. & Pinnaduwage, L. A. (1999, Oct. 5-8). Dissociative electron attachment to laser-excited benzene. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Zhu, Y. & Pinnaduwage, L. A. (1997, Oct. 6-9). Long-time stability of superexcited high Rydberg molecular states. 50th Annual Gaseous Electronics Conference. Madison, WI.

Publication Type: Proceeding

Pinnaduwage, L. A, Ding, W. X., & McCorkle, D. L. (1998, Jun. 27 - Jul. 3). Enhanced electron attachment to superexcited Rydberg states of molecular hydrogen using a plasma mixing scheme. Presented at the 1998 International Congress on Plasma Physics. Prague, Czech Republic.

Pinnaduwage, L. A. (1997, Jun. 29 - Jul. 2). Implications of electron attachment to highly-excited states in pulsed power discharges. 11th IEEE Pulsed Power Conference. Baltimore, MA.

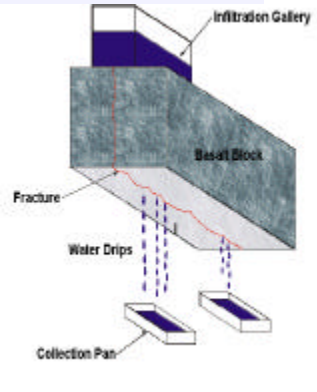


Illustration of the infiltration test design at the Hell's Half Acre site, Idaho, to investigate a key problem of infiltration in fractured rocks - water dripping through fractures. [see Project #55359]

Project: 55359

Title: Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone

PI: Dr. Boris Faybishenko

Institution: Lawrence Berkeley National Laboratory

Publication Type: Journal

Finsterle, S. & Faybishenko, B. (1999). Design and analysis of an experiment to determine hydraulic parameters of variably saturated porous media. Advances in Water Resources, 22(1),431-444.

Publication Type: Presentation

Carrigan, C. R, et. al. (1999). Lessons on transport and monitoring from the LLNL Vadose Zone Observatory. Proceedings of the 1999 Spring AGU Meeting. Boston, MA.

Faybishenko, B. & Finsterle, S. (1999). On the physics of tensiometry in heterogeneous soils and rocks. Proceedings of the 1999 Spring AGU Meeting. Boston, MA.

Faybishenko, B. (1998, May). Theory and numerical evaluation of the parameters of the chaotic behavior of flow in unsaturated soils and rocks. Chapman Conference on Fractal Scaling, Non-Linear Dynamics, and Chaos in Hydrologic Systems. Clemson University. Clemson, SC.

Faybishenko, B. (1998, Oct.). A fuzzy-chaotic analysis of water flow and chemi-

cal transport in unsaturated-saturated soils. 16th World Congress of Soil Science. Montpellier, France.

Faybishenko, B. (Ed.) (1999, Feb. 10-12), Proceedings of the International Symposium Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. Berkeley, CA.

Faybishenko, B., et. al. (1997). Conceptual model of geometry and physics of liquid flow in unsaturated fractured basalt at Box Canyon Site. Proceedings of the 1997 Fall Meeting of AGU. San Francisco, CA.

Faybishenko, B., et. al. (1998). Multi-scale investigations of flow in fractured rocks. Proceedings of the 1998 Fall Meeting of AGU. San Francisco, CA. F377-378.

Faybishenko, B., Wood, T. R., Stoops, T. M., Doughty, C., & Jacobsen, J. (1997). A conceptual model of tracer transport in fractured basalt: Large Scale Infiltration Test revisited. Proceedings of 1997 GSA Annual Conference. Salt Lake City, UT.

Geller, J. T., Borglin, S. E., & Faybishenko, B. (1998, May). Experimental study and evaluation of dripping water in fracture models. Chapman Conference on Fractal Scaling, Non-Linear Dynamics, and Chaos in Hydrologic Systems. Clemson University. Clemson, SC.

Geller, J. T., Borglin, S. E., & Faybishenko, B. (1998). Experimental study and evaluation of dripping water in fracture models. Proceedings of the 1998 Fall Meeting of AGU. San Francisco, CA. F383.

Publication Type: Press release

Faybishenko, B. (1999, Dec. 17). Water travels chaotically through the ground. A Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone (see Web site: http: //www.eurekalert.org/releases/ineel-wtcttg.html).

Publication Type: Proceeding

Faybishenko, B. (1999). Comparison of laboratory and field methods for determination of unsaturated hydraulic conductivity of soils. LBNL Report-42022. Proceedings of the International Conference - Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media.

Faybishenko, B. (1999). Evidence of chaotic behavior in flow through fractured rocks, and how we might use chaos theory in fractured rock hydrogeology. In Proceedings of the International Symposium Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. Berkeley, CA. 207-212.

Finsterle, S. & Faybishenko, B. (1998). What does a tensiometer measure in fractured rocks? LBNL Report-41454. Proceedings of the International Conference - Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media.

Nikravesh, M., Cox, L., Faybishenko, B., & Aminzadeh, F. (1999, Mar.). Characterization of contaminated sites using sparse well data. SPE Paper 49330.

Podgorney, R. K. & Wood, T. R. (1999). Observations of water movement in variably saturated fractured basalt and its possible implications on predictive modeling. In Proceedings of the International Symposium Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances. Berkeley, CA. 300-304.

Publication Type: Report

Babchin, A. J., Faybishenko, B., Sivashinsky, G. I., Frenkel, A., & Halpern, D. (1999). A model of chaotic time evolution of a slow liquid film on an inclined plane: One-dimensional solution. LBNL Report 42884.

Benito, P., Cook, P., Faybishenko, B., Freifeld, B., & Doughty, C. (1999). Box canyon air-connectivity study. Preliminary Data Analysis, LBNL Report 42359.

Faybishenko, B., et al. (1997). A chaotic-dynamical conceptual model to describe fluid flow and contaminant transport in a fractured vadose zone. In Environmental Management Science Program Awards Fiscal Year 1997 Annual Report Progress. Lawrence Berkeley National Laboratory Report, LBNL-41192.

Faybishenko, B., et. al. (1997). A chaotic-dynamical conceptual model to describe fluid flow and contaminant transport in a fractured vadose zone. 1997 Anual Report. Report No. LBNL-41223.

Podgorney, R. K., Wood, T. R., & Stoops, T. M. (1998). Basalt outcrop infiltration tests to evaluate chaotic behavior of unsaturated flow in fractured rock. INEEL Data Summary Report 1997 Field Season.

Podgorney, R. K., Wood, T. R., & Stoops, T. M. (1999). Basalt outcrop infiltration tests to evaluate chaotic behavior of unsaturated flow in fractured rock. INEEL Data Summary Report 1998 Field Season.

Project: 55367

Title: Investigation of Microscopic Radiation Damage in Waste Forms Using ODNMR and AEM Techniques

PI: Dr. Guokui Liu *Institution:* Argonne National Laboratory

Publication Type: Journal

Liu, G. K., Li, S. T., Beitz, J. V., & Abraham, M. M. (1998). J. Alloys & Compounds, 271/273,872.

Publication Type: Proceeding

G. K. Liu, et. al. (1998). Scientific basis for nuclear waste management XXI. MRS Sym. Pro. V506, 921.

Project: 55380

Title: In-Situ Spectro-Electrochemical Studies of Radionuclide Contaminated Surface Films on Metals and the Mechanism of their Formation and Dissolution

PI: Dr. Carlos A. Melendres *Institution:* Argonne National Laboratory

Publication Type: Paper

Carlos, A. (1999, Apr. 5). X-ray absorption spectroscopy studies of electrochemically deposited thin oxide films. Materials Research Society Spring Meeting.

Melendres, C. A. (1999, May 3). X-ray absorption spectroscopy studies of the structure of electrodeposited metal oxide films and some applications. 193rd Meeting of the Electrochemical Society.

Project: 55388

Title: Stable Isotopic Investigations of In Situ Bioremediation of Chlorinated Organic Solvents

PI: Dr. Neil C. Sturchio *Institution:* Argonne National Laboratory

Publication Type: Journal

Heraty, L. J., Fuller, M. E., Huang, L., Abrajano, T., & Sturchio, N. C. (1999, in press). Carbon and chlorine isotopic fractionation during microbial degradation of dichloromethane. Organic Geochemistry.

Holt, B. D., Sturchio, N. C., Abrajano, T. A., & Heraty, L. J. (1997, in press). Conversion of chlorinated organic compounds to carbon dioxide and methyl chloride for isotopic analysis of carbon and chlorine. Analytical Chemistry 69,2727-2733.

Huang, L., Sturchio, N. C., Abrajano, T., Heraty, L. J., & Holt, B. D. (1999, in press). Comparison of C and Cl isotope fractionation of chlorinated aliphatic hydrocarbons during evaporation and biodegradation. Organic Geochemistry.

Sturchio, N. C., et. al. (1998, in press). Stable chlorine isotope investigation of natural attenuation of trichloroethene in an aerobic aquifer. Environmental Science and Technology 32,3037-3042.

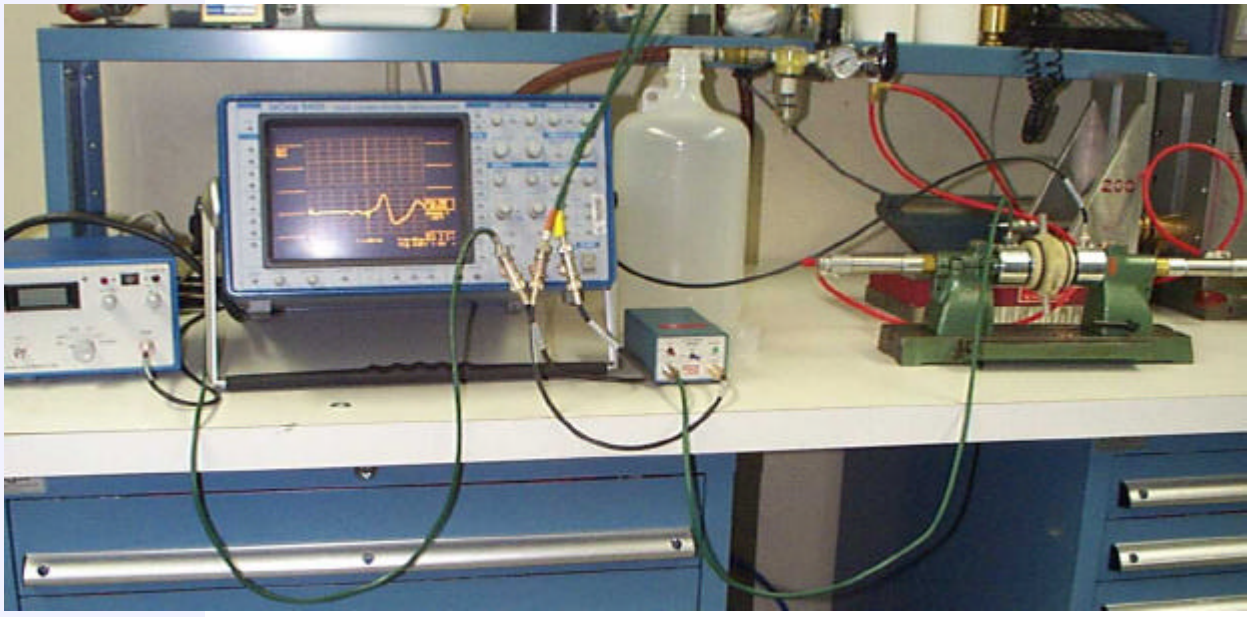
Project: 55395

Title: Physics of DNAPL Migration and Remediation in the Presence of Heterogeneities

PI: Dr. Stephen H. Conrad *Institution:* Sandia National Laboratories

Publication Type: Report

Borchers, B., Conrad, S. H., Webb, E. K., Glass Jr., R. J., Cox, R. (1997). A simulation and decision analysis approach to locating DNAPL in subsurface sediments. Sandia Report SAND97-2261.



Photograph of experimental apparatus for measuring ultrasonic compressional and shear wave velocities in soils at low pressures. The oscilloscope screen displays an amplified signal from the pulse generator at the far left. This signal travelled through the soil sample in the sample holder assembly to the right. [see Project #55411]

Project: 55411

Title: Joint Inversion of Geophysical Data for Site Characterization and Restoration Monitoring

PI: Dr. Patricia A. Berge *Institution:* Lawrence Livermore National Laboratory

Publication Type: Journal

Berryman, J. G. & Pride, S. R. (1998). Volume averaging, effective stress rules, and inversion for microstructural response of multicomponent porous media. LLNL report UCRL-JC-127248, Int. J. Sol. Struct., 35,4811-4843.

Pride, S. R. & Berryman, J. G. (1998). Connecting theory to experiment in poroelasticity. J. Mech. Phys. Sol., 46,719-747.

Publication Type: Paper

Berryman, J. G. & Berge, P. A. (1999, Mar. 24-27). Mixture theory for predicting geomechanical coefficients of heterogeneous reservoirs. Fifth Society for Industrial and Applied Mathematics (SIAM) Conference on Mathematical and Computational Issues in the Geosciences. San Antonio, TX. 110.

Publication Type: Patent

Berryman, J.G. (1999). Robust discrimination of porosity and fluid saturation using seismic velocity analysis. DOE Patent Docket No. S-92015, LLNL Patent disclosure IL-10437.

Bonner, B. P., Boro, C., & Hart, D. J. (1999, Apr.). Anti-waveguide for ultrasonic testing of granular media under elevated stress. LLNL Patent disclosure.

Publication Type: Proceeding

Berge, P. A., Bonner, B. P., Aracne-Ruddle, C., Trombino, C., & Berryman, J. G. (1999). Compressional and shear wave velocities of soils at low pressures—Theoretical estimates, and comparison of laboratory and field data. LLNL report UCRL-JC-133211 Abs, Proceedings of the Seismological Society of America (SSA) 94th Annual Meeting, Seismological Research Letters, 70,226.

Bonner, B. P., et. al. (1999, Mar. 14-18). Ultrasonic characterization of synthetic soils for application to near surface geophysics. In Powers, M. H., Cramer, L., & Bell, R. S. (Eds.), Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Oakland, CA. Environmental and Engineering Geophysical Society. Wheat Ridge, CO. 455-463.

Publication Type: Report

Aracne-Ruddle, C., Wildenschild, D., Bonner, B., & Berge, P. (1998). Direct observation of morphology of sand-clay mixtures with implications for mechanical properties in sediments. LLNL report UCRL-JC-131702 Abs, Eos, Transactions of the American Geophysical Union, 79, Fall Meeting Supplement, F820.

Aracne-Ruddle, C., Wildenschild, D., Bonner, B., & Berge, P. (1998, Oct. 15-16). Direct observation of fluid-clay interactions with implications for mechanical and electrical properties. LLNL report UCRL-JC-131116 Abs. Presentation at the LLNL Women's Technical and Professional Symposium. San Ramon, CA.

Berge, P. A. & Berryman, J. G. (1999, Mar. 24-27). Developing rock physics algorithms for velocity-porosity relations with environmental geophysics applications. LLNL report UCRL-JC-132054 Abs, Fifth Society for Industrial and Applied Mathematics (SIAM) Conference on Mathematical and Computational Issues in the Geosciences. San Antonio, TX. 108.

Berge, P. A., Berryman, J. G., Bonner, B. P., Roberts, J. J., & Wildenschild, D. (1999, Mar. 14-18). Comparing geophysical measurements to theoretical estimates for soil mixtures at low pressures. LLNL report UCRL-JC-132893. In Powers, M. H., Cramer, L., & Bell, R. S. (Eds.), Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP), Oakland, CA. Environmental and Engineering Geophysical Society. Wheat Ridge, CO. 465-472.

Berge, P. A., Berryman, J. G., Bonner, B. P., Roberts, J. J., & Wildenschild, D. (1998, Oct. 15-16). Preliminary results from an environmental geophysics Project for improving geophysical imaging of fluid distribution in the shallow subsurface. LLNL report UCRL-JC-131209 Abs. Presentation at the LLNL Women's Technical and Professional Symposium. San Ramon, CA.

Berge, P. A., Berryman, J. G., Roberts, J. J., & Wildenschild, D. (1998, Jul. 27-30). Joint inversion of geophysical data for site characterization and restoration monitoring. EMSP Project summary/progress report for FY98 for EMSP Project 55411. LLNL report UCRL-JC-128343, presented at the DOE Environmental Management Science Workshop, Chicago, IL.

Berge, P. A., Berryman, J. G., Roberts, J. J., & Wildenschild, D. (1997). Joint inversion of geophysical data for site characterization and restoration monitoring. In Carrigan, C. R. & Jackson, K. J. (Eds.), Environmental Management Science Program: Fiscal Year 1997 Progress Report, Lawrence Livermore National Laboratory (LLNL) report UCRL-ID-129562, LLNL, Livermore, CA.

Berryman, J., Dvorkin, J., Le Ravalec, M., & Nur, A. (1997). Effective moduli of particulates with elastic cement. LLNL report UCRL-JC-128340.

Bonner, B. P., Hart, D. J., Berge, P. A., & Aracne, C. M. (1997). Influence of chemistry on physical properties: Ultrasonic velocities in mixtures of sand and swelling clay. LLNL report UCRL-JC-128306abs, Eos, Transactions of the American Geophysical Union, 78, Fall Meeting Supplement, F679.

Rowe, C. D. (1997, summer). Joint inversion of geophysical data for site characterization and restoration monitoring. In Williams, B. (Ed.), The Associated Western Universities Summer Participant Program at the Lawrence Livermore National Laboratory, Summer 1997: LLNL report UCRL-ID-128721-97, LLNL. Livermore, CA. 75-78.

Trombino, C. N. (1998). Elastic properties of sand-peat moss mixtures from ultrasonic measurements. LLNL report UCRL-JC-131770. LLNL, Livermore, CA.

Wildenschild, D., Roberts, J. J. & Carlberg, E. D. (1998). Transport and microstructural properties of sand-clay mixtures. LLNL report UCRL-JC-131703 Abs, Eos, Transactions of the American Geophysical Union, 79, Fall Meeting Supplement, F820.

Wildenschild, D., Roberts, J. J., & Carlberg, E. (1999, Mar. 14-18). Influence of microstructural properties on geophysical measurements in sand-clay mixtures. LLNL report UCRL-JC-131557. In Powers, M. H., Cramer, L., & Bell, R.S. (Eds.), Proceedings of the Symposium on the Application of Geophysics to Engineering and Environmental Problems (SAGEEP). Oakland, CA. Environmental and Engineering Geophysical Society. Wheat Ridge, CO. 445-454.

Project: 55416

Title: Control of Biologically Active Degradation Zones by Vertical Heterogeneity: Applications in Fractured Media

PI: Dr. Frederick S. Colwell *Institution:* Idaho National Engineering and Environmental Laboratory

Publication Type: Poster

Colwell, F. S. (1999, Jan. 15). Control of biologically active degradation zones by vertical heterogeneity: Applications in fractured media. NABIR Investigator's Workshop.

Publication Type: Presentation

Colwell, F. S. (1999). Chaotic-dynamical conceptual model to describe fluid flow and contaminant transport in a fractured vadose zone. Poster presentation at the Berkeley Dynamics of Fluids and Fractured Rock Conference. Berkeley, CA.

Colwell, F. S., Tobin, K., & Wilson, M. (1999, Jan. 7). Control of biologically active degradation zones by vertical heterogeneity: Applications in fractured media. Idaho Water Resources Research Institute (IWRRI) meeting.

Project: 59786

Title: Design and Construction of *Deinococcus radiodurans* for Biodegradation of Organic Toxins at Radioactive DOE Waste Sites

PI: Dr. Michael J. Daly *Institution:* Uniformed Services Univ. of the Health Sciences

Publication Type: Journal

Lange, C., Wackett, L., Minton, K. & Daly, M. J. (1998). Engineering a recombinant Deinococcus radiodurans for organopollutant degradation in radioactive mixed waste environments. Nature Biotech., 16,929-933.

Project: 59827

Title: The Influence of Radiation and Multivalent Cation Additions on Phase Separation and Crystallization of Glass

PI: Dr. Michael C. Weinberg *Institution:* University of Arizona

Publication Type: Paper

Jeoung, J. S., Poisl, W. H., Weinberg, M. C., Smith, G. L., & Li, H. (1999). Effect of iron oxidation state on immiscibility temperature in sodium silicate glass. Amer. Ceram. Soc. Bull. 78(4), 205.

Project: 59828

Title: Bioavailability of Organic Solvents in Soils: Input into Biologically Based Dose-Response Models for Human Risk Assessments

PI: Dr. Ronald C. Wester *Institution:* University of California at San Francisco

Publication Type: Journal

Poet, T. S., Corley, R. A , Thrall, K. D., & Wester, R. C. (1999). Assessing the dermal bioavailability of volatile organics in rats. The Toxicologist, 48,339.

Wester, R. C., et. al. (1999). An innovative method to detemrine dermal uptake of solvents from soil and water in vivo in humans. The Toxicologist, 48,338.

Publication Type: Other

Thrall, K. D., Poet, T. S., & Corley, R. A. (1998). An innovative method to determine percutaneous absorption: Real time breath analysis and physiologically based pharmacokinetic modeling. In Bronaugh, R. & Maibach, H. (Eds.), Percutaneous Absorption, Third Edition, Marcel Dekker, Inc. New York, NY.

Publication Type: Presentation

Wester, R. C. (1998). Chemical manufactures association workshop of research planning. Research Triangle Park, NC.

Wester, R. C. (1998, Sept.). Dermal bioavailability. Presetation at NIOSH, Morgantown, WV.

Wester, R. C. (1999, Oct.). 15th Annual International Conference on Contaminated Soils and Water. University of Massachusetts. Amherst, MA.

Project: 59849

Title: Radionuclide Immobilization in the Phases Formed by Corrosion of Spent Nuclear Fuel: The Long-Term Assessment

PI: Dr. Rodney C. Ewing *Institution:* University of Michigan

Publication Type: Journal

Casas, I., et. al. (1998). The role of pe, pH, and carbonate on the solubility of UO2 and uraninite under nominally reducing conditions. Geochimica et Cosmochimica Acta 62(13),2223-2231.

Chen, F., Burns, P. C., & Ewing, R. C. (1999). 79-Se: Geochemical and crystallochemical retardation mechanisms. Journal of Nuclear Materials, 275, 81-94.

Chen, F., Ewing, R. C., & Clark, S. B. (1999). The Gibbs free energies and enthalpies of formation of uranium (VI) phases: An empirical method of prediction. American Mineralogist 84(4),650-654.

Fayek, M., Burns, P., Guo, Y. -X., & Ewing, R. C. (1999, in press). Microstructures associated with uraninite alteration. Journal of Nuclear Materials.

Finch, R. J., Cooper, M. A., Hawthorne, F. C., & Ewing, R. C. (1999, in press). Refinement of the crystal structure of rutherfordine. Canadian Mineralogist.

Publication Type: Presentation

Ewing, R. C. (1999, Sept. 26 - Oct. 1). Results of uranyl phase analyses. Presented at the Seventh International Conference on the Chemistry and Migration Behavior of Actinides and Fission Products in the Geosphere. Lake Tahoe, CA.

Publication Type: Proceeding

Chen, F. & Ewing, R. C. (1999, in press). 79-Se geochemical and crystallochemical retardation mechanisms. Proceedings of the Materials Research Society.

Chen, F. & Ewing, R. C. (1999, in press). Structural contributions to the third-law entropies of uranyl phases. Proceedings of the Materials Research Society.

Project: 59882

Title: Measurements of Radon, Thoron, Isotopic Uranium and Thorium to Determine Occupational & Environmental Exposure & Risk at Fernald Feed Materials Production Center.

PI: Dr. Naomi H. Harley *Institution:* New York University Medical School

Publication Type: Presentation

Harley, N. H. (1999, Jun.). Field results of personal radon and thoron monitor. Annual Health Physics Meeting. Philadelphia, PA. Health Physics 76,163.

Harley, N. H. (1999, Jun.). Results of particle size sampler field tests. Annual Health Physics Meeting. Philadelphia, PA. Health Physics 76,163.

Project: 59918

Title: Improved Radiation Dosimetry/Risk Estimates to Facilitate Environmental Management of Plutonium Contaminated Sites

PI: Dr. Bobby R. Scott *Institution:* Lovelace Biomedical & Environmental Research Institute

Publication Type: Journal

Cheng, Y. -S., Zhou, Y., & Chen, B. T. (1999, in press). Particle deposition in a cast of human oral airways. Aerosol Science & Technology.

Hoover, M. D., & Newton, G. J. (1998). Performance testing of continuous air monitors for alpha-emitting radionuclides. Radiat. Prot. Dosim., 79(1-4),499-504.

Hoover, M. D., et. al. (1998). Characterization of enriched uranium dioxide particles from a uranium handling facility. Radiat. Prot. Dos., 79(1-4),57-62.

Hoover, M. D., Mewhinney, C. J., & Newton, G. J. (1999). Modular glovebox connector and associated good practices for control of radioactive and chemically toxic materials. Health Phys. 76(1),66-72.

Hoover, M. D., Mewhinney, C. J., & Newton, G. J. (1999). Modular glovebox connector and associated good practices for control of radioactive and chemically toxic materials. Health Phys., 76(1),66-72.

Osovets, S. V. & Scott, B. R. (1998, Mar. 6). Nonmonotonous character of dose-response relationships. Viniti No. ¼, 645, B98 (in Russian).

Scott, B. R. & Fencl, A. (1999, in press). Variability in PuO2 intake by inhalation: Implications for DOE worker protection. Radiat. Prot. Dosim.

Scott, B. R. (1999). Evaluating the risk of death via the Hematopoietic syndrome mode from prolonged exposure of nuclear workers to radiation delivered at very low raters. Health Physics 74,545-553.

Scott, B. R. (1999). Transformation of C3H 10T1/2 cells. Letter to Editor, J. Radiol. Prot. 19(2),177-179.

Scott, B. R. (1999). Variability in PuO2 intake by inhalation: Implications for worker protection at the U.S. Department of Energy. Radiation Protection Dosimetry. 83(3),221-232.

Scott, B. R., Lyzlov, A. F., & Osovets, S. V. (1998). Evaluating the risk of death via the hematopoietic syndrome mode for prolonged exposure of nuclear workers to radiation delivered at very low rates. Health Physics 74 (5),545-553.

Publication Type: Other

Glissmeyer, J. A., et. al. (1999). American national standard for sampling and monitoring releases of airborne radioactive substances from the stacks and ducts of nuclear facilities. ANSI/HPS N13.1-1999, Health Physics Society, McLean, VA.

Guilmette, R. A. & Scott, B. R. (1998.) Radiation toxicology. In Wexler, P. (Ed.), Encyclopedia of Toxicology, 3,5-18. Academic Press. San Diego, CA.

Publication Type: Poster

Scott, B. R., Hoover, M. D., Neft, R. E., & Fencl, A. F. (1999, Aug. 22-26). Recommendations for improving the interim radionuclide soil action levels for the Rocky Flats Cleanup Agreement. Poster presentation at the 218th American Chemical Society National Meeting. New Orleans, LA.

Publication Type: Presentation

Cheng, Y. -S., Yeh, H. C., Smith, S. M., Cheng, K. H., & Swift, D. L. (1998, Sept. 14-18). Deposition of ultrafine particles in the nasal and tracheobronchial airways. 1998 International Aerosol Conference. Edinburgh, UK.

Hoover, M. D. (1998, Apr. 24). Workplace air sampling methods and good practices. Technical Workshop on Air Sampling: The Big Picture. Savannah River Chapter, Health Physics Society. Aiken, SC.

Hoover, M. D. (1998, Jul. 12). Statistical considerations for aerosol sampling, professional enrichment short course. 43rd Annual Meeting of the Health Physics Society. Minneapolis, MN.

Hoover, M. D. (1999, Jan. 24). Statistical considerations for aerosol sampling. Professional Enrichment Short Course. 32nd Midyear Meeting of the Health Physics Society. Albuquerque, NM.

Hoover, M. D. (1999, Jan. 24). Statistical considerations for aerosol sampling. Professional Enrichment Short Course. 32nd Midyear Meeting of the Health Physics Society. Albuquerque, NM.

Hoover, M. D., Newton, G. J., & Cox, F. M. (1998, Feb. 7). Sampling radioactive aerosols. American Academy of Health Physics Short Course. 31st Midyear Meeting of the Health Physics Society. Mobile, AL.

Hoover, M. D., Newton, G. J., & Cox, F. M. (1998, Jul. 15). Flow measurements with rotameters and appropriate corrections. 43rd Annual Meeting of the Health Physics Society. Minneapolis, MN.

Scott, B. R. (1998, Aug.). Improved radiation dosimetry/risk estimates to facilitate environmental management of plutonium contaminated sites. Presentation at the American Chemical Society. New Orleans, LA.

Scott, B. R., et. al. (1998, Jul. 27-30). Evaluating the intake via inhalation of plutonium oxides for the stochastic exposure paradigm. Poster 13 presented at the Environmental Management Science Program Workshop. Chicago, IL.

Smith, S. M., Cheng, Y. S., & Yeh, H. C. (1998, Sept. 14-18). Diffusional deposition of ultrafine particles in human tracheobronchial airways. 1998 International Aerosol Conference, Edinburgh, UK.

Zhang, Z., Wang, X., & Cheng, Y. -S. (1998, Sept. 14-18). Flow pattern and aerosol deposition in the human oral airway. 1998 International Aerosol Conference, Edinburgh, UK.

Publication Type: Proceeding

Glissmeyer, J. A., et. al. (1999). American national standard for sampling and monitoring releases of airborne radioactive substances from the stacks and ducts of nuclear facilities. ANSI/HPS N13.1-1999, Health Physics Society. McLean, VA.

Scott, B. R. (1998). Improved radiation dosimetry/risk estimates to facilitate environmental management of plutonium contaminated sites. In Environmental Management Science Program Workshop, U. S. Department of Energy Publication CONF-980736. Washington, D. C. 25-26.

Project: 59925

Title: Modeling of Diffusion of Plutonium in Other Metals and of Gaseous Species in Plutonium-Based Systems

PI: Dr. Bernard R. Cooper *Institution:* West Virginia University

Publication Type: Journal

Cooper, B. R., Becker, J. D., Wills, J. M., & Cox, L. (1998). Calculated lattice relaxation in Pu-Ga. Phys. Rev. B 58B,5143.

Cooper, B. R., Becker, J. D., Wills, J. M., & Cox, L. (1998). Calculated lattice relaxation in Pu-Ga alloys. Journal of Alloys and Compounds, 271-273,367.

Cooper, B. R., Vogt, O., Sheng, Q.G., & Lin, Y.L. (1999, May). From heavy fermions to random-localized-site behavior via Anderson localization. Philosophical Magazine B 79, No. 5,683-702.

Publication Type: Other

Cooper, B. R., Turchi, P.E.A., Gonis, A., Kioussis, N., & Price, D. L. (1999). Correlation effects on stability in Pu metal and its alloys. In Gonis, A. & Kioussis, N. (Eds.), Electron Correlations and Materials Properties. Plenum Publishing.

Publication Type: Presentation

Cooper, B. R. & Beiden, S. (1998). Diffusion of plutonium into transition metallic alloys and of transition metal species into plutonium. Eighth Conference on Computational Research on Materials. Lakeview, WV.

Cooper, B. R. & Beiden, S. (1998). Modeling of diffusion of plutonium in other metals and of gaseous species in plutonium-based systems. Environmental Management Science Workshop. Chicago, IL.

Cooper, B. R. & Beiden, S. (1998, Nov.). Modeling of diffusion of plutonium. Workshop on Environmental Management Science: Integration with End User Needs. Savannah River Site. Aiken, SC.

Cooper, B. R. & Beiden, S. (1998, Nov.). Modeling of interdiffusion of plutonium and other metals. Materials Research Society Meeting. Boston, MA.

Cooper, B. R. & Lederman, D. (1998, Nov.). Portable detection and analysis of plutonium content. Workshop on Environmental Management Science: Integration with End User Needs. Savannah River Site. Aiken, SC.

Cooper, B. R. (1998, Jun. 28 - Jul. 3). Synthesis of many-body theory and electronic structure. International Workshop on Electron Correlations and Materials Properties. Heraklion, Crete, Greece.

Cooper, B. R. (1998, May). Treating electronic and magnetic properties of actinide-based materials beyond one-electron dynamics. School of Actinide Physics and Chemistry. Uppsala, Sweden.

Cooper, B. R. (1999, Apr.). Random 5f localization and the fcc transition and depression of melting temperature in plutonium. 29th Journees des Actinides Conference. Luso, Portugal.

Cooper, B. R. (1999, Mar.). Anomalous electronic behavior and relationship to thermostructural behavior of light actinides. American Physical Society Meeting. Atlanta, GA.

Cooper, B. R., Becker, J. D., Wills, J. M. & Cox, L. (1997, Sept.). Structural relaxation in Pu-Ga via full-potential LMTO calculations. Actinides 97. International Conference. Baden-Baden, Germany.

Cooper, B. R., Kioussis, N., Turchi, P. E. A., Gonis, A., & Price, D. L. (1999, Mar.). Electronic structure of alpha and delta plutonium. American Physical Society Meeting. Atlanta, GA.

Cooper, B. R., Sevilla, E. H., & Fernando, G. W. (1999, Mar.). Equilibrium lattice volume of fcc Pu. American Physical Society Meeting. Atlanta, GA.

Project: 59934

Title: Hazardous Gas Production by Alpha Particles in Solid Organic Transuranic Waste Matrices

PI: Dr. Jay A. LaVerne *Institution:* University of Notre Dame

Publication Type: Journal

Chang, Z. & LaVerne, J. A. (1999, in press). Molecular hydrogen production in the radiolysis of high density polyethylene. J. Phys. Chem.

Publication Type: Presentation

LaVerne, J. A. & Chang, Z. (1999, Aug. 23). Hydrogen production in the radiolysis of polyethylene. 218th ACS National Meeting. New Orleans, LA.

Project: 59960

Title: Direct Investigations of the Immobilization of Radionuclides in the Alteration Phases of Spent Nuclear Fuel

PI: Dr. Peter C. Burns *Institution:* University of Notre Dame

Publication Type: Journal

Burns, P. C. & Finch, R.J. (1999, in press). Wyartite: crystallographic evidence for the first pentavalent-uranium mineral. American Mineralogist.

Burns, P. C. & Hill, F. C. (1998, in press). Implications of the synthesis and structure of the Sr analogue of curite. Canadian Mineralogist.

Burns, P. C. (1998). The structure of boltwoodite and implications of solid-solution towards sodium boltwoodite. Canadian Mineralogist 36,1069-1075.

Burns, P. C. (1998). The structure of compreignacite, K2[(UO2)3O2(OH)3]2(H2O)7. Canadian Mineralogist 36,1061-1067.

Burns, P. C. (1999. Cs boltwoodite obtained by ion exchange from single crystals: Implications for radionuclide release in a nuclear repository. Journal of Nuclear Materials 265,218-223.

Chen, F., Burns, P.C., & Ewing, R.C. (1999, in press). 79 Se: Geochemical and crystallo-chemical retardation mechanisms. Journal of Nuclear Materials.

Hill, F.C. & Burns, P.C. (1999, in press). Structure of a synthetic Cs uranyl oxide hydrate and its relationship to compreignacite. Canadian Mineralogist.

Publication Type: Paper

Burns, P. C. (1999, in press). The crystal chemistry of uranium. Mineralogical Society of America Reviews in Mineralogy.

Publication Type: Presentation

Burns, P. C. & Finch, R. J. (1999). The structure of wyartite: Crystallographic evidence for the first pentavalent-uranium mineral. GAC-MAC. Sudbury, Ontario, Canada.

Burns, P. C. (1998): Topological aspects of uranyl mineral structures. IMA. Toronto, Canada.

Burns, P. C., Finch, R. C. & Wronkiewicz, D. J. (1998). Direct investigations of the immobilization of radionuclides in the alteration products of spent nuclear fuel. DOE Environmental Management Science Program Workshop. Chicago, IL.

Hill, F. C. & Burns, P. C. (1998). Chemical and structural diversity in the uranyl oxide hydrate system. GSA Toronto, Canada.

Hill, F. C. & Burns, P. C. (1998). Investigations of the crystal chemistry of uranyl oxide hydrates. IMA Toronto, Canada.

Hill, F. C. & Burns, P. C. (1999). The importance of uranyl silicates for the disposal of nuclear waste. GAC-MAC. Sudbury, Ontario, Canada.

Kim, C. W. & Wronkiewicz, D. J. (1998). Alteration phases of spent nuclear fuel. Missouri Academy of Sciences, 1998 Annual Meeting.

Publication Type: Proceeding

Chen, F., Burns, P.C., & Ewing, R.C. (1998, in press). 79-Se: Geochemical and crystallo-chemical retardation mechanisms. The Scientific Basis for Nuclear Waste Management XX. MRS Proceedings.

Project: 59967

Title: Aqueous Electrochemical Mechanisms in Actinide Residue Processing
PI: Dr. David E. Morris *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Morris, D. E. (1998, Jul. 27-30). Aqueous electrochemical mechanisms in actinide residue processing. DOE Environmental Management Science Program Workshop. Chicago, IL.

Morris, D. E. (1999, Apr. 21-25). Trends in actinyl electrochemistry: Voltammetry and theory. Presentation at the 217th National Meeting of the American Chemical Society. Anaheim, CA.

Morris, D. E. (1999, Aug. 22-26). Aqueous electrochemical mechanisms in actinide residue processing results. Presentation at the National Meeting of the American Chemical Society. New Orleans, LA.

Morris, D. E. (1999, Aug. 22-26). Aqueous electrochemical mechanisms in mediated dissolution of actinide residues. First Accomplishments of Environmental Management Science Program. National Meeting of the American Chemical Society. New Orleans, LA.

Project: 59977

Title: Synthesis and Characterization of Templated Ion Exchange Resins for the Selective Complexation of Actinide Ions
PI: Dr. George M. Murray *Institution:* Johns Hopkins University Applied Physics Lab

Publication Type: Journal

Bae, S. Y., Southard, G. L., & Murray, G. M., (1999, in press). Molecularly imprinted ion exchange resin for purification, preconcentration and determination of UO2 2+ by spectrophotometry and plasma spectrometry. Analytica Chimica Acta.

Publication Type: Paper

Arnold, B. R., Jenkins, A. L., Uy, O. M., & Murray, G. M. (1999). Progress in the development of molecularly imprinted polymer sensors. JHUAPL Technical Digest, 20,190-198.

Publication Type: Presentation

Kimaro, A. & Murray, G. M. (1998, Mar. 7-12). Synthesis and characterization of templated ion exchange resins for the selective complexation of actinide ions. Abstract No. 2315P, Pittsburgh Conference. Orlando, FL.

Project: 59978

Title: Thermospray Mass Spectrometry Ionization Processes Fundamental Mechanisms for Speciation, Separation and Characterization of Organic Complexants in DOE Wastes

PI: Dr. John E. Caton *Institution:* Oak Ridge National Laboratory

Publication Type: Presentation

Bostick, D. (1999, Aug. 22-26). Separation and speciation of organic complexants in DOE wastes using HPLC on zirconia based stationary phases and thermospray mass spectrometry. Presentation at the National Meeting of the American Chemical Society. New Orleans, LA.

Bostick, D. (1999, Nov. 16). HPLC separation of chelating agents on quaternized polyethyleneimine coated zirconia. Eastern Analytical Symposium. Monchanin, DE.

Project: 59981

Title: Real-Time Broad Spectrum Characterization of Hazardous Waste by Membrane Introduction Mass Spectrometry

PI: Dr. Charles W. Wilkerson, *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Wilkerson Jr., C. W. (1999, Feb. 22-23). Workshop on harsh environment mass spectrometry. St. Petersburg, FL.

Wilkerson Jr., C. W. (1999, Feb. 28 - Mar. 4). WM99 - HLW, LLW, mixed wastes and environmental restoration - Working towards a cleaner environment. Tucson, AZ.

Wilkerson Jr., C. W. (1999, Mar. 7-12). Pittsburgh conference on analytical chemistry and applied spectroscopy. Orlando, FL.

Project: 59982

Title: Reactivity of Peroxynitrite: Implications for Hanford Waste Management and Remediation

PI: Dr. Sergei V. Lymar *Institution:* Brookhaven National Laboratory

Publication Type: Journal

Coddington, J. W., Hurst, J. K., & Lymar, S. V. (1999). Hydroxyl radical formation during peroxynitrous acid decomposition. J. Am. Chem. Soc., 121,2438-2443.

Coddington, J. W., Wherland, S., & Hurst J. K. (1999). Radical intermediates in peroxynitrite reactions. Nitric Oxide, 3,37.

Czapski, G., Lymar, S. V., & Schwarz, H. A. (1999). Acidity of the carbonate radical. J. Phys. Chem. A, 103,3447-3450.

Gerasimov, O. V. & Lymar, S. V. (1999). Pathways of decomposition and one-electron oxidation by peroxynitrous acid. Nitric Oxide, 3,7.

Goldstein, S., Saha, A., Lymar, S. V., & Czapski, G. (1998). Oxidation of peroxynitrite by inorganic radicals: A pulse radiolysis study. J. Am. Chem. Soc., 120,5549-5554.

Lymar, S. V. & Hurst, J. K. (1998). ACO 2 -catalyzed one-electron oxidations by peroxynitrite: Properties of the reactive intermediate. Inorganic Chemistry, 37,294-301.

Lymar, S. V. & Hurst, J. K. (1998). Radical nature of peroxynitrite reactivity. Chem. Res.Toxicol., 11,714-715.

Project: 59990

Title: Fundamental Chemistry, Characterization, and Separation of Technetium Complexes in Hanford Waste

PI: Dr. Norman C. Schroeder *Institution:* Los Alamos National Laboratory

Publication Type: Other

Schroeder, N. C., Radzinski, S. D., Ashley, K. R., Truong, A. P., & Szczepaniak, P. A. (1998). Technetium oxidation state adjustment for hanford waste processing. In Lombardo, N. J. & Schulz, W. W. (Eds.), Science and Technology for Disposal of Radioactive Tank Waste. Plenum Publishing Corporation. New York, NY.

Publication Type: Proceeding

Ashley, K. R., Whitener, G. D., Schroeder, N. C., Ball, J. R., & Radzinski, S. D. (1999). In Bond, A. H., Dietz, M. L. & Rogers, R. D. (Eds.), Progress in Metal Ion Separation and Preconcentration, ACS Symposium Series 716, American Chemical Society, Washington, D. C. 219.

Project: 60017

Title: Removal of Technetium, Carbon Tetrachloride, and Metals from DOE Properties

PI: Dr. Thomas E. Mallouk *Institution:* Pennsylvania State University

Publication Type: Proceeding

Ponder, S. M., Ford, J. R., Darab, J. G., & Mallouk, T. E. (1999, in press). Ferragels: A new family of materials for remediation of aqueous metal ion solutions. MRS Symp. Proceedings.

Project: 60020

Title: Stability of High-Level Waste Forms

PI: Dr. Theodore M. Besmann *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Besmann, T. M., Beahm, E. C., & Spear, K. E. (1999). An approach to thermochemical modeling of nuclear waste glass. In Marra, J. C. & Chandler, G. T. (Eds.), Environmental Issues and Waste Management Technologies IV, 277-87. Ceramic Transactions, 93, American Ceramic Society. Westerville, OH.

Besmann, T. M., Beahm, E. C., & Spear, K. E. (1999, in press). An approach to thermochemical modeling of nuclear waste glass. In Marra, J. C. & Chandler, G. T. (Eds.), Environmental Issues and Waste Management Technologies IV, 277-87. Ceramic Transactions, 93, American Ceramic Society. Westerville, OH.

Spear, K. E., Besmann, T. M., & Beahm, E. C. (1999, Apr.). Thermochemical modeling of glass: Application to high-level nuclear waste glass. MRS Bulletin, 37-44.

Spear, K. E., Bessman, T. M., & Beahm, E. C. (1999, Apr.). Thermochemical modeling of glass: Application to high-level nuclear waste glass. MRS Bulletin, 37-44.

Project: 60037

Title: Estimation of Potential Population Level Effects of Contaminants on Wildlife

PI: Ms. Linda Mann *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Mann, L. (1999, in press). Allometric models for interspecies extrapolation of wildlife toxicity data. Bulletin of Environmental Contamination and Toxicology.

Publication Type: Poster

Sample, B. E., Arenal, C. A., & Mann, L. K. (1999). Determination of sensitivity of birds and mammals to environmental contamination. Poster presentation at the SETAC annual meeting.

Project: 60070

Title: The Development of Cavity Ringdown Spectroscopy as a Sensitive Continuous Emission Monitor for Metals

PI: Dr. George P. Miller *Institution:* Mississippi State University

Publication Type: Journal

Miller, G. P. & Winstead, C. B. (1997). Inductively coupled plasma cavity ringdown spectroscopy. J. Anal. Atomic Spectro., 12,907.

Winstead, C. B., Mazzotti, F. J., Mierzwa, J., & Miller, G. P. (1999, in press). Preliminary results for electrothermal atomization - cavity ringdown spectroscopy (ETA-CRDS). Anal. Comm.

Publication Type: Presentation

Miller, G. P. & Winstead, C. B. (1997, Jan. 12-17). ICP-cavity ringdown spectroscopy. Abstract O1-4, Winter Conference in Spectrochemistry. Gent, Belgium.

Miller, G. P. & Winstead, C. B. (1998, Oct. 12-15). ICP-cavity ringdown spectroscopy. Abstract 407, The 25th FACSS Conf. Austin, TX.

Project: 60075

Title: Particle Generation by Laser Ablation in Support of Chemical Analysis of High Level Mixed Waste from Plutonium Production Operations

PI: Dr. J. Thomas Dickinson *Institution:* Washington State University

Publication Type: Paper

Dickinson, J. T. (1998, Aug.). Mechanisms for and characterization of particulate generation by laser irradiation of inorganic crystalline materials. DOE-EMSP Workshop on Waste Characterization. Chicago, IL.

Dickinson, J. T. (1998, Jun.). Ejection of droplets and fracture particles from single crystal NaNO 3 during pulsed laser irradiation. Gordon Research Conference on Laser Interaction with Materials.

Dickinson, J. T. (1999, Jun.). UV laser interactions with inorganic single crystals with molecular anions. American Chemical Society. Portland, OR.

Dickinson, J. T. (1999, Mar.). High energy ions from UV laser irradiation of cleaved ionic crystals. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, Mar.). Laser desorption of energetic ions from single crystal NaNO 3 at 1064 nm. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, Mar.). The effect of surface treatment on excimer laser induced positive ion desorption in brushite. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, Mar.). Ultrafast and nanosecond laser induced desorption from ionic solids. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, May). Laser-induced positive ion and neutral atom/ molecule emission from single crystal CaHPO 4 2H 2 O: The role of radiation induced defects. Materials Research Society. San Francisco, CA.

Dickinson, J. T. (1999, May). Studies of particulate formation by laser ablation in support of chemical analysis of high level mixed waste. American Ceramics Society. Indianapolis, IN.

Hedges, A. L., Mendoza, A., Alexander, M. L., Langford, S.C., & Dickinson, J. T. (1999, Mar.) Investigations of particle formation by laser ablation for elemental analysis. 217th ACS meeting. Anaheim, CA.

Publication Type: Presentation

Alexander, M. L., Langford, S. C., & Dickinson, J. T. (1998, Oct.). Fundamental mechanisms of particulate formation by laser ablation for inductively coupled plasma mass spectrometry (LA/ICP-MS). Presentation at the SPIE East conference. Boston, MA.

Alexander, M. L., Langford, S.C., & Dickinson, J. T. (1999, Mar.). Particle generation by laser ablation in support of chemical analysis of high level mixed waste from plutonium production operations. Invited presentation at the DOE Characterization and Monitoring Sensor Technology (CMST) meeting. Gaithersburg, MD.

Dickinson, J, T. (1999, Jan.). The desorption of energetic ions from ionic crystals. Dept. of Physics, Washington State University. Pullman, WA.

Dickinson, J. T. (1998, Jun.). The laser desorption of ions from ionic crystals. Gordon Conference on Laser Materials Interactions.

Dickinson, J. T. (1998, Nov.). New models of laser desorption and particle formation. Physics Dept. Colloquium. University of Linz, Austria.

Dickinson, J. T. (1998, Oct. - Nov.). Topics in surface dynamics. Guest Lecturer, Institute of Applied Physics. University of Linz, Austria.

Dickinson, J. T. (1998, Oct.). Mechanisms for and characterization of particulate generation by laser irradiation of inorganic crystalline materials. FACS National Meeting. Austin TX.

Dickinson, J. T. (1999, Jan.). The use of lasers in chemical analysis. University of Minho. Braga, Portugal.

Dickinson, J. T. (1999, Jun.). Laser desorption and chemical analysis. Departments of Physics and Chemistry. U. of Heidelberg, Germany.

Dickinson, J. T. (1999, Jun.). The laser desorption of ions from ionic crystals. E-MRS Symposium on Laser Materials Interactions. Strasbourg, France.

Dickinson, J. T. (1999, Jun.). The use of lasers in chemical analysis of toxic materials. Paul Scherrer Institute. Villigen PSI, Switzerland.

Project: 60096

Title: Rational Synthesis of Imprinted Organofunctional Sol-Gel Materials for Toxic Metal Separation

PI: Dr. Ziling Benjamin Xue *Institution:* University of Tennessee at Knoxville

Publication Type: Journal

Dai, S., et. al. (1999). Imprint coating: Novel synthesis of selective functionalized ordered mesoporous sorbents. Angew. Chem. Int. Ed., 38,1235-1239.

Dai, S., et. al. (1999, in press). A new methodology to functionalize surfaces of ordered mesoporous materials based on ion exchange reactions. Adv. Mater.

Shin, Y. S., Burleigh, M. C., Dai, S., Barnes, C. E., & Xue, Z. L. (1999). Investigation of uranyl adsorption on mesoporous titanium-based sorbents. Radiochim. Acta. 84,37-42.

Project: 60115

Title: Advanced High Resolution Seismic Imaging, Material Properties Estimation and Full Wavefield Inversion for the Shallow Subsurface

PI: Dr. Alan Levander *Institution:* Rice University

Publication Type: Journal

Zelt, C. A., Hojka, A. M., Flueh, E. R., & McIntosh, K. D. (1999, in press). 3D simultaneous seismic refraction and reflection tomography of wide-angledata from the central Chilean margin. Geophys. Res. Lett.

Zelt, C. A., Optimal utilization of sub-optimal 3D wide-angle data. Seis. Res. Lett., 70,255.

Publication Type: Presentation

Akerberg, P., Dana, D., Levander, A., Zelt, C., & Henstock, T. (1998). High resolution shallow seismic imaging at an open pit copper mine. 10th Annual IRIS Workshop. Santa Cruz, CA.

Dana, D., Akerberg, P., Levander, A., Zelt, C., & Henstock, T. J. (1998). Shallow-seismic investigation at an open pit copper mine: A comparison with drill data. EOS, Trans. Am. Geophys. Union, 79,F652.

Dana, D., Akerberg, P., Zelt, C., Levander, A., & Henstock, T. (1998). High resolution seismic imaging at a porphyry copper mine. Society of Exploration Geophysicists. New Orleans, LA.

Dana, D., Zelt, C., & Levander, A. (1999). High-resolution seismic survey over a near-surface contamination site. SEG International Exposition and Sixty-Ninth Annual Meeting.

Passmore, P., Keller, G. R., Miller, K. C., Levander, A., & McMechan, G. (1999). Single-channel recorder test results from two different active source experiments. Seism. Res. Letters, 70,243.

Zelt, C. A. & Hojka, A. M. (1998). 3D simultaneous seismic refraction and reflection tomography of wide-angle traveltime data from the central Chilean margin. EOS, 79,F638.

Project: 60118

Title: Fundamental Thermodynamics of Actinide-Bearing Mineral Waste Forms
PI: Dr. Mark A. Williamson *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Putnam, R. L., Navrotsky, A., Cordfunke, E. H. P., & Huntelaar, M. E. (1999, in press). Thermodynamics of formation for two cerium aluminum oxides, CeAlO3 and CeAl12O19.918, and cerium sesquioxide, Ce2O3 at T= 298.15 K. J. Chem. Thermodynamics.

Putnam, R. L., Navrotsky, A., Woodfield, B. F., & Boerio-Goates, J. (1999). Heat capacity, third law entropy, and formation energetics of zirconolite, CaZrTi2O7. Environmental Issues and Waste Management Technologies in the Ceramic and Nuclear Industries IV, Ceramic Transactions, 93,339.

Putnam, R. L., Navrotsky, A., Woodfield, B. F., Boerio-Goates, J., & Shapiro, J. L. (1999). Thermodynamics of formation of zirconolite (CaZrTi2O7) from T = 298.15 K to T = 1500 K. J. Chem. Thermo. 31,229-243.

Putnam, R. L., Navrotsky, A., Woodfield, B. F., Boerio-Goates, J., & Shapiro, J. L. (1999). Thermodynamics of formation for zirconolite, CaZrTi2O7, From T= 298 K to T= 1500 K, J. Chem. Thermodynamics 31(3),229.

Putnam, R. L., Navrotsky, A., Woodfield, B. F., Shapiro, J. L., & Boerio-Goates, J. (1999). Heat capacity, third law entropy, and formation energetics of zirconolite, CaZrTi2O7. In Marra, J. C. & Chandler, G. T. (Eds.), Environmental Issues and Waste Management Technologies in the Ceramic and Nuclear Industries IV, Ceramic Transactions, 93. The American Ceramic Society. Westerville, OH.

Woodfield, B. F., Boerio-Goates, J., Shapiro, J. L., Putnam, R. L., & Navrotsky, A. (1999). Molar heat capacity and thermodynamic functions of zirconolite, CaZrTi2O7. J. Chem. Thermodynamics 31(3),245.

Woodfield, B. F., Boerio-Goates, J., Shapiro, J. L., Putnam, R. L., & Navrotsky, A. (1999). Molar heat capacity and thermodynamic functions of zirconolite, CaZrTi2O7. J. Chem. Thermo. 31,245-253.

Woodfield, B. F., et. al. (1999, in press). Molar heat capacity and thermodynamic functions for CaTiO3. Journal of Chem. Thermo.

Woodfield, B. F., et. al. (1999, in press). Molar heat capacity and thermodynamic functions for CaTiO3. J. Chem. Thermodynamics.

Woodfield, B. F., et. al. (1999, in press). Molar heat capacity and thermodynamic functions for CaTiO3. J. Chem. Thermodynamics.

Publication Type: Other

Putnam, R. L., Ph.D. Dissertation. (1999, Nov.). Department of Geosciences, Princeton University, NJ.

Publication Type: Presentation

Putnam, R. L., et. al., (1998, Dec.). Thermochemistry of Hf-zirconolite, CaHfTi2O7. Scientific Basis for Nuclear Waste Management, Materials Research Society.

Publication Type: Proceeding

Putnam, R. L., et. al. (1999, in press). Thermochemistry of Hf-zirconolite, CaHfTi2O7. MRS Proceedings.

Project: 60123

Title: Potential-Modulated Intercalation of Alkali Cations into Metal Hexacyanoferrate Coated Electrodes
PI: Dr. Daniel T. Schwartz *Institution:* University of Washington

Publication Type: Journal

Haight, S. M., Schwartz, D. T., & Lilga, M. A. (1999). In-situ oxidation state profiling of nickel hexacyanoferrate derivatized electrodes using line-imaging Raman spectroscopy and multivariate calibration. J. Electrochem. Soc. 146,1866.

Project: 60144

Title: Flow Visualization of Forced and Natural Convection in Internal Cavities
PI: Dr. John C. Crepeau *Institution:* University of Idaho

Publication Type: Paper

McCreery, G. E., et. al. (1999, Sept. 6-9). Flow visualization of forced convection in fuel storage canisters. Presentation at the ANS Global ’99 International Conference on Future Nuclear Systems.

McCreery, G.E., et. al. (1999, Aug.). Flow visualization of forced and natural convection in fuel storage canisters. Presentaion at the Global 99 International Conference on Future Nuclear Systems.

Project: 60150

Title: Genetic Engineering of a Radiation-Resistant Bacterium for Biodegradation of Mixed Wastes

PI: Dr. Mary E. Lidstrom *Institution:* University of Washington

Publication Type: Poster

Meima, R., Rothfuss, H., Gewin, L., & Lidstrom, M. E. (1998, Jul. 27-30). Genetic engineering of a radiation-resistant bacterium for biodegradation of mixed wastes. Poster presentation at the DOE Environmental Management Science Program Workshop. Chicago, IL.

Project: 60155

Title: Measurements and Models for Hazardous Chemical and Mixed Wastes

PI: Dr. Cynthia Holcomb *Institution:* National Institute of Standards & Technology - Boulder

Publication Type: Journal

Mathias, P. M., Naheiri, T., & Oh, E. M. (1989). A density correction for the Peng-Robinson equation of state. Fluid Phase Equilibria, 47,77-87.

Project: 60158

Title: Development of Radon-222 as a Natural Tracer for Monitoring the Remediation of NAPL Contamination in the Subsurface

PI: Dr. Lewis Semprini *Institution:* Oregon State University

Publication Type: Other

Semprini, L., Cantaloub, M., Gottipati, S., Hopkins, O., & Istok, J. (1998). Radon-222 as a natural tracer for quantifying and monitoring NAPL remediation. In Wickramanayake, G. B. & Hinchee, R. E. (Eds.), Nonaqueous-phase Liquids: Remediation of Chlorinated and Recalcitrant Compounds. Battelle Press, Columbus, OH. 137-142.

Publication Type: Presentation

Cantaloub, M. (1998, Nov. 16-19). The role of cocktail solvent on radon measurement by liquid scintillation analysis. Packard Instrument Co. Environmental LSC Workshop at the 44th Annual Conference on Bioassay, Analytical, and Environmental Radiochemistry. Albuquerque, NM.

Cantaloub, M., Higginbotham, J., Istok, J. & Semprini, L. (1998, Nov. 16-19). Interaction of sample, cocktail and headspace volume when measuring aqueous Rn in small volume samples. 44th Annual Conference on Bioassay, Analytical, and Environmental Radiochemistry. Albuquerque, NM.

Cantaloub, M., Humphrey, M., Istok, J., & Semprini, L. (1998, Dec. 6-10). Monitoring NAPL remediation using Rn-222 as an in-situ indicator. 1998 Fall Meeting of the American Geophysical Union. San Francisco, CA.

Cantaloub, M., Istok, J., & Semprini, L. (1998, Dec. 1-3). Radon-222 as a natural tracer for monitoring the remediation of NAPL contamination in the subsurface. Strategic Environmental Research and Development Program (SERDP) and Environmental Security Technology Certification Program (ESTCP) Technical Symposium and Workshop. Arlington, VA.

Cantaloub, M., Istok, J., & Semprini, L. (1998, Jul. 20-23). Investigations of Radon-222 as an internal tracer for monitoring NAPL remediation. Symposium on Environmental Models and Experiments Envisioning Tomorrow; Behavior and Remediation of Nonaqueous Phase Liquid Contaminants in the Subsurface. UC Irvine, CA.

Cantaloub, M., Istok, J., & Semprini, L. (1998, Oct. 20-23). Site assessment and remediation monitoring using naturally occuring Rn-222. The 5th International Petroleum Environmental Conference. Albuquerque, NM.

Semprini, L., Istok, J., & Cantaloub, M. (1998, Jul. 27-30). Development of Rn-222 as a tracer for monitoring the remediation of NAPL contamination in the subsurface. Department of Energy Environmental Management Science Program Scientific Workshop, Rosemont, IL.

Project: 60162

Title: Enhancements to & Characterization of the Very Early Time Electromagnetic (VETEM) Prototype Instrument & Applications to Shallow Subsurface Imaging at Sites in the DOE Complex

PI: Dr. David L. Wright *Institution:* U.S. Geological Survey - Denver

Publication Type: Journal

Cui, T. J. & Chew, W. C. (1999, in press). Modeling of arbitrary wire antennas above ground. IEEE Trans. on Geoscience and Remote Sensing.

Cui, T. J. & Chew, W. C. (1999, Jun.). Fast algorithm for electromagnetic scattering by buried conducting plates of large size. IEEE Trans. on Antennas and Propagation, 47(6),1116-1118.

Cui, T. J. & Chew, W. C. (1999, Mar.). Fast evaluation of sommerfeld integrals for EM scattering and radiation by three-dimensional buried objects. IEEE Trans. on Geoscience and Remote Sensing, GE-37(2),887-900.

Cui, T. J. & Chew, W. C. (1999, Sept.). Fast algorithm for electromagnetic scattering by buried 3D dielectric objects of large size. IEEE Trans. on Geoscience and Remote Sensing, GE-37(5),2597-2608.

Publication Type: Paper

Cui, T. J. & Chew, W. C. (1999, Aug. 15-22). Fast algorithm for electromagnetic scattering by buried 3D dielectric objects of large size. XXVIth General Assembly of the International Union of Radio science, 982. Toronto, Canada.

Cui, T. J. & Chew, W. C. (1999, Jul. 12-15). Accurate model of arbitrary wire antennas in free space, above or inside ground. Digest of IEEE Antennas and Propagation Society International Symposium, 2, 982-985. Orlando, FL.

Wright, D. L. et. al. (1999, Aug. 13-21). An assessment of the prototype very early time electromagnetic system (VETEM). XXVIth General Assembly of the International Union of Radio science. Toronto, Canada.

Wright, D. L., et. al. (1999, Mar. 14-18). New field and modeling results from a simulated waste pit using the enhanced very early time electromagnetic (VETEM) prototype system. Proceeding of the 12th Annual Symposium on the Applications of Geophysics to Environmental and Engineering Problem (SAGEEP), Oakland, CA.

Publication Type: Report

Cui, T. J. & Chew, W. C. (1999, Aug.). Novel difraction tomographic algorithm for imaging two-dimensional dielectric objects buried under a lossy earth. Research Report, Electromagnetics Laboratory, University of Illinois at Urbana-Champaign. No. CCEM-21-99. Also submitted to IEEE Trans. on Geoscience and Remote Sensing.

Cui, T. J. & Chew, W. C. (1999, Jan.). Accurate model of arbitrary wire antennas in free space, above or inside ground. Electromagnetics Laboratory, University of Illinois at Urbana-Champaign, Research Report No. CCEM-2-99. Also submitted to IEEE Trans. on Antennas and Propagation.

Cui, T. J. & Chew, W. C. (1999, Jul.). Frequency-spatial domain inverse scattering of two-dimensional dielectric objects buried under a lossy earth. Research Report, Electromagnetics Laboratory, University of Illinois at Urbana-Champaign. No. CCEM-19-99. Also submitted to IEEE Trans. on Microwave Theory and Techniques.

Cui, T. J., et. al. (1999, Mar.). Numerical modeling of an enhanced very early time electromagnetic (VETEM) prototype system. Research Report, Electromagnetics Laboratory, University of Illinois at Urbana-Champaign. No. CCEM-7-99. Also submitted to IEEE Antennas and Propagation Magazine.

Cui, T. J., et. al. (1999, May). Nonlinear inverse scattering of two-dimensional dielectric objects buried under a lossy earth. Research Report, Electromagnetics Laboratory, University of Illinois at Urbana-Champaign. No. CCEM-12-99. Also submitted to IEEE Trans. on Geoscience and Remote Sensing.

Project: 60163

Title: Investigation of Techniques to Improve Continuous Air Monitors Under Conditions of High Dust Loading in Environmental Settings

PI: Dr. Stephen D. Schery *Institution:* New Mexico Institute of Mining & Technology

Publication Type: Presentation

Rodgers, J. C., Wasiolek, P. T., Schery, S. D., & Alcantara, R. E. (1998, Nov. 1-6). High resolution real-time optical studies of radiological air sample processes in an environmental continuous air monitor. 1998 SPIA Symposium on Industrial and Environmental Monitors and Biosensors. Boston, MA. LA-UR-98-1684.

Project: 60199

Title: Seismic-Reflection and Ground Penetrating Radar for Environmental Site Characterization

PI: Dr. Don W. Steeples *Institution:* University of Kansas

Publication Type: Journal

Baker, G. S., Schmeissner, C., Steeples, D. W., & Plumb, R. G. (1999). Seismic reflections from depths of less than two meters. Geophys. Res. Lett., 26(2),279-282.

Baker, G. S., Steeples, D. W., & Schmeissner, C. (1999). In-situ, high-frequency P-Wave velocity measurements within 1 m of the Earth's surface. Geophysics, 64(2),323-325.

Steeples, D. W. & Baker, G. S. (1998, Jun.). Near-surface contributions to seismic static corrections. AAPG Explorer, 19, 20-21,29.

Steeples, D. W., Baker, G. S., & Schmeissner, C. (1999). Toward the autojuggie: Planting 72 geophones in 2 seconds, Geophysical Research Letters, 26(8),1085-1088.

Steeples, D. W., Baker, G. S., Schmeissner, C., & Macy, B. K. (1999). Geophones on a board. Geophysics, 64(3),809-814.

Publication Type: Other

Baker, G. S., Ph D. Dissertaion. (1999, May). Seismic imaging shallower than three meters. The University of Kansas, Lawrence, KS.

Publication Type: Poster

Plumb, R. G., Steeples, D. W., Baker, G. W., Schmeissner, C., & Pavlovic, M. (1999, Jun.). A combined ground-penetrating radar and shallow seismic reflection approach to characterizing hydrological flow. International Geoscience and Remote Sensing Society (IGARSS) meeting. Hamburg, Germany.

Publication Type: Presentation

Baker, G. S., Plumb, R. G., Steeples, D. W., Pavlovic, M., & Schmeissner, C. (1998). Coincident GPR and ultrashallow seismic imaging in the Arkansas River Valley, Great Bend, Kansas. SEG Expanded Abstracts, SEG 1998 International Meeting. New Orleans, LA. 859-861.

Baker, G. S., Steeples, D. W., Schmeissner, C., & Macy, B. K. (1998). In-situ, high-resolution P-wave velocity measurements within 1 m of the Earth's surface. SEG Exp. Abstr., SEG 1998 International Meeting. New Orleans, LA. 856-858.

Steeples, D. W., Baker, G. S., & Schmeissner, C. (1998, Dec. 6-10). Toward the autojuggie: Planting 72 geophones in 2 seconds. (1998). American Geophysical Union, 1998 Fall Meeting. San Francisco, CA.

Steeples, D. W., Baker, G. S., Schmeissner, C., & Macy, B. K. (1998). Geophones on a board. SEG Exp. Abstr., SEG 1998 International Meeting. New Orleans, LA. 852-855.

Project: 60217

Title: Optically-Based Array Sensors for Selective in Situ Analysis of Tank Waste
PI: Dr. Gilbert M. Brown *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Ji, H. -F., Brown, G. M., & Dabestani, R. (1999). Calix[4]arene-based Cs+ selective optical sensor. Chem. Comm., 609.

Ji, H. -F., Dabestani, R., Brown, G. M., & Hettich, R. L. (1999). Spacer length effect on the photoinduced electron transfer fluorescent probe for alkali metal ions. Photochem. Photobiol. 69,513.

Publication Type: Presentation

Ji, H. -F., Dabestani, R., & Brown, G. M. (1998, Aug.). Fluorescence probes for the detection of potassium ions. Presentation at the American Chemical Society National Meeting. Boston, MA.

Project: 60218

Title: Novel Mass Spectrometry Mutation Screening for Contaminant Impact Analysis
PI: Dr. C. H. Winston Chen *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Golovlev, V. V., Allman , S. L., Garrett, W. R., Taranenko, N. I., & Chen, C. H. (1997). Laser induced acoustic desorption. International Journal of Mass Spectrometry and Ion Processes, 169/170,69-78.

Taranenko, N. I., Allman, S. L., Golovlev, V. V., & Chen, C. H. (1999, in press). Chemical cleavage sequencing of DNA using matrix-assisted laser desorption/ ionization time-of-flight mass spectrometry. Analytical Chemistry.

Taranenko, N. I., et. al. (1998). Matrix-assisted laser desorption/ionization for short tandem repeat loci. Rapid Comm. Mass Spectrom., 12,413-418.

Taranenko, N. I., et. al. (1998). Sequencing DNA using mass spectrometry for ladder detection. Nucleic Acids Research, 26(10),2488-2490.

Project: 60219

Title: Development of Advanced Electrochemical Emission Spectroscopy for Monitoring Corrosion in Simulated DOE Liquid Waste
PI: Dr. Digby D. MacDonald *Institution:* Pennsylvania State University

Publication Type: Presentation

Sikora, E. & Macdonald, D. D. (1999, May 9-15). Passive films on iron formed in the presence of EDTA. Presentation at the 8th International Symposium on Passivity of Metals and Semiconductors. Jasper, Canada.

Project: 60231

Title: Novel Miniature Spectrometer for Remote Chemical Detection
PI: Dr. Andrew C. R. Pipino *Institution:* National Institute of Standards & Technology - Maryland

Publication Type: Journal

Pipino, A. C. R. (1998, Nov.). Evanescent wave cavity ring-down spectroscopy for ultra-sensitive chemical detection. SPIE 3535,57. Boston, MA.

Pipino, A. C. R., et. al. (1997). Evanescent wave cavity ring-down spectroscopy with a total-internal-reflection minicavity. Rev. Sci. Instrum., 68,2978.

Pipino, A.C.R., et. al. (1997). Evanescent wave cavity ring-down spectroscopy as a probe of surface processes. Chem. Phys. Lett., 280,104.

Project: 60271

Title: Characterization of a New Family of Metal Transport Proteins
PI: Dr. Mary Lou Guerinot *Institution:* Dartmouth College

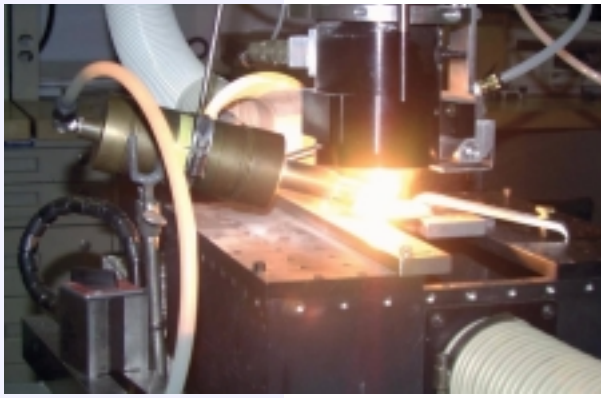
Publication Type: Journal

Eng, B. H., Guerinot, M. L., Eide, D., & Saier, M. H. J. (1998). Sequence analyses and phylogenetic characterization of the ZIP family of metal ion transport proteins. J. Membr. Biol., 166,1-7.

Gitan, R. S., Luo, H., Rodgers, J., Broderius, M., & Eide, D. (1998). Zinc-induced inactivation of the yeast ZRT1 zinc transporter occurs through endocytosis and vacuolar degradation. J. Biol. Chem., 273, 28617-28624.

Guerinot, M. L. & Eide, D. (1999). Zeroing in on zinc uptake in yeast and plants. Curr. Opin. Plant Biol., 2, 244-249.

Korshunova, Y. O., Eide, D., Clark, W. G., Guerinot,
M. L., & Pakrasi, H. B. (1999). The IRT1 protein from Arabidopsis thaliana is a metal transporter with broad specificity. Plant Mol. Biol., 40,37-44.



Laser Ablation System – 1.6 kw pulsed Nd:YAG laser system with fiber optic beam delivery. Advantages of this system over conventional scabbling are for hard-to-reach places and remote decontamination. [see Project #60283]

Project: 60283

Title: Waste Volume Reduction Using Surface Characterization and Decontamination by Laser Ablation
PI: Dr. Michael J. Pellin
Institution: Argonne National Laboratory

Publication Type: Poster

Savina, M. R., Pellin, M. J., Leong, K., & Xu, Z. (1998, Jul.). Waste volume reduction using surface characterization and decontamination by laser ablation. Presentation at EMSP Workshop. Rosemont, IL.

Publication Type: Presentation

Pellin, M. J., Savina, M. R., Reed, C. B., Wang, Y., & Xu, Z. (1999, Mar.). Waste volume reduction using surface characterization and decontamination by laser ablation. Presentation at Characterization, Monitoring, and Sensing Workshop. Gaithersburg, MD.

Publication Type: Proceeding

Savina, M. R., Xu, Z., Wang, Y., Leong, K., & Pellin, M. J. (1998). Laser ablation of concrete. Proceedings of the 17th International Conference on Applications of Lasers and Electro-Optics, 85A,219-226.

Project: 60296

Title: Research Program to Investigate the Fundamental Chemistry of Technetium
PI: Dr. Norman M. Edelstein *Institution:* Lawrence Berkeley National Laboratory

Publication Type: Presentation

Edelstein, N. M. (1999, Sept. 22-25). Technetium chemistry in highly basic solutions. Presentation at the Technetium Chemistry Workshop. Hanford, WA.

Project: 60313

Title: Radiation Effects on Transport and Bubble Formation in Silicate Glasses
PI: Dr. Alexander D. Trifunac *Institution:* Argonne National Laboratory

Publication Type: Journal

Shkrob, I. A., Tadjikov, B. M., Chemerisov, S. D. & Trifunac, A. D. (1999). Electron trapping and hydrogen atoms in oxide glasses. J. Chem. Phys., 111,5124-5140.

Project: 60328

Title: High Frequency Electromagnetic Impedance Measurements for Characterization, Monitoring and Verification Efforts

PI: Dr. Ki-Ha Lee *Institution:* Lawrence Berkeley National Laboratory

Publication Type: Report

Frangos, W. & Becker, A. (1998). Magnetic fields of AM band radio broadcast signals at the Richmond Field Station. Lawrence Berkeley National Lab Report LBNL-42654.

Lee, K. H. (1997). High-frequency electric field measurement using a toroidal antenna. Lawrence Berkeley National Lab Report LBNL-39894, UC-2040.

Project: 60345

Title: New Silicotitanate Waste Forms: Development and Characterization

PI: Dr. Mari Lou Balmer *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Nyman M., et. al. (1999, in press). Synthesis and characterization of a new microporous Cs-Ti-Si-O-H2O ion exchanger. Chemistry of Materials.

Nyman, M., et. al. (1999, in press). Synthesis and characterization of Cs2TiSi4O11: A novel durable phase with potential waste form applications. Chemistry of Materials.

Publication Type: Presentation

Balmer, M. L. (1999). Results on phases a, b (Si, Ti phases) and e, f (Niobate phases). United Engineering Foundations: Metals Separations for 2000 and beyond.

Balmer, M. L., et. al. (1999, Apr. 25-28). Ceramic wasteforms from Cs-loaded crystalline silicotitanates. 101th Annual Meeting of the American Ceramic Society. Indianapolis, IN.

Nyman, M. D. & Nenoff, T. M. (1999, Jun.). Selective inorganic crystalline ion exchange materials for cesium and strontium. United Engineering Foundation and AIChE.

Nyman, M. D., et. al. (1998). CSTs: Stability and use as alternative waste forms. Mat. Res. Soc. Fall Meeting.

Nyman, M. D., et. al. (1999). Hydrothermal synthesis of Cs-Ti-Si-O phases as alternative waste forms for Cs-loaded CST ion exchangers. 1999 Spring American Chemical Society meeting. Anaheim, CA.

Su, Y., et. al. (1998). Evaluation of thermally converted silicotitanate waste forms II. Mat. Res. Soc. Fall Meeting.

Su, Y., et. al. (1998). Evaluation of thermally converted silicotitanate waste forms II. Proc. Mat. Res. Soc.

Xu, H., et. al. (1999, Apr. 25-28). Thermo-chemistry of crystalline silicotitanate phases in the Cs2O-Na2O-SiO2-TiO2-H2O system. 101st Annual Meeting of the American Ceramic Society. Indianapolis, IN.

Publication Type: Proceeding

Nyman, M. D., et. al. (1998). CSTs: Stability and use as alternative waste forms. Proc. Mat. Res. Soc. Fall Meeting.

Project: 60355

Title: Mineral Surface Processes Responsible for the Decreased Retardation (or Enhanced Mobilization) of ^{137}Cs from HLW Tank Discharges

PI: Dr. John M. Zachara *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Zachara, J. M. (1999, Aug.). New advances in the understanding of 137Cs interactions with micas and implications to Cs geochemistry in the Hanford vadose zone. Keynote address given to the EMSP National Program Workshop. Chicago, IL.

Project: 60387

Title: Distribution & Solubility of Radionuclides & Neutron Absorbers in Waste Forms for Disposition of Plutonium Ash & Scraps, Excess Plutonium, and Misc. Spent Nuclear Fuels

PI: Dr. Denis M. Strachan *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Gu, B. X., Wang, L. M., & Ewing, R. C. (1999, in press). The effect of amorphization on the Cs ion exchange and retention capacity of zeolite-NaY. Journal of Nuclear Materials.

Li, L., Strachan, D. M., Li, H., Davis, L. L., & Qian, M. (1999, in press). Peraluminous and peralkaline effects on Gd2O3 and La2O3 solubilities in sodium-alumino-borosilicate glasses. Ceramic Transactions. American Ceramic Society. Westerville, OH.

Zhao, D., et. al. (1999, in press). Electron microprobe and electron microscopy characterization of precipitated gadolinium crystals in borosilicate glasses. Journal of Non-Crystalline Solids.

Publication Type: Other

Feng, X., et. al. (1999). Distribution and solubility of radionuclides in waste forms for disposition of plutonium and spent nuclear fuels: Preliminary results. In Marra, J. C. & Chandler, G. T. (Eds.), Ceramic Transactions, 93,409-419. American Ceramic Society, Westerville, OH.

Publication Type: Presentation

Davis, L. L., et. al. (1998, Dec.). The effects of Na2O, Al2O3, and B2O3 on HfO2 solubility in borosilicate glass. Materials Research Society, Boston, MA.

Feng, X. (1998, Mar. 17). A plasma arc-vitreous ceramic process for stabilizing EBR-II spent nuclear fuels. National Academy of Science.

Feng, X., et. al. (1998, May). Distribution and solubility of radionuclides in waste forms for disposition of plutonium and spent nuclear fuels: Preliminary results. Symposium of Waste Management Science and Technology in the Ceramic and Nuclear Industries. 100th Am. Cer. Soc. Annual Meeting. Cincinnati, OH.

Li, L., Strachan, D. M., Davis, L. L., Li, H., & Qian, M. (1998, Dec.). Gadolinium solubility limits in sodium-alumino-borosilicate glasses. Materials Research Society Meeting. Boston, MA.

Li, L., Strachan, D. M., Li, H., Davis, L. L., & Qian, M. (1999, Apr. 24-29). Peraluminous and peralkaline effects on Gd2O3 and La2O3 solubilities in sodium-alumino-borosilicate glasses. American Ceramic Society Meeting. Indianapolis, IN.

Shuh, D. K., et. al. (1998, Jul. 28). Distribution and solubility of radionuclides and neutron absorbers in forms for disposition of plutonium ash and scraps, excess plutonium, and miscellaneous spent nuclear fuels. Environmental Management Science Program Workshop Plenary Address. Chicago, IL.

Shuh, D. K., et. al. (1998, Jul. 9). Investigations of actinide materials chemistry utilizing synchrotron radiation methods. Chemical and Analytical Sciences Division, Oak Ridge National Laboratory. Oak Ridge, TN.

Stachan, D. M. (1999, Jun. 1). The Yucca Mountain repository: What has changed? American Geophysical Union, Spring meeting. Boston, MA.

Strachan, D. M. (1999, Apr. 22). Radiation effects in ABO4 orthophosphates and orthosilicates. Invited presentation at theHLW and Pu Immobilization Workshop. CEA, Saclay, France.

Strachan, D. M. (1999, Apr. 5). Performance assessments: The design, selection and importance of nuclear waste forms. Invited presentation at Ch Performance Assessments: The Design, Selection and Importance of Nuclear Waste Forms.

Strachan, D. M. (1999, Jul. 12). Ageing studies of nuclear waste forms: The evaluation of long-term behaviour. Plenary lecture for International Conference on Ageing Studies & Lifetime Extension of Materials, St. Catherine's College. Oxford, United Kingdom.

Strachan, D. M. (1999, Oct. 20). Natural systems: Applications to nuclear waste management. Invited presentation at workshop sponsored by the Russian Academy of Sciences and the U.S. Department of Energy. Moscow, Russia.

Strachan, D. M. (1999, Sept. 10). Radiation effects in zircon. Invited seminar at the Université Henri Poincaré. Nancy, France.

Vance, E. R., et. al. (1999, Apr. 28). Crystal chemistry, radiation effects and aqueous leaching of brannerite, UTi2O6. S-I-059-99, Materials Division, ANSTO, Menai, NSW 2234, Australia.

Publication Type: Proceeding

Davis, L. L., et. al. (1998). The effects of Na2O, Al2O3, and B2O3 on HfO2 solubility in borosilicate glass. In Scientific Basis for Nuclear Waste Management XXII. Materials Research Society. Pittsburgh, PA.

Ewing, R. C. (1999, in press). Ageing studies of nuclear waste forms: The evaluation of long-term behaviour. Proceedings of International Conference on Ageing Studies & Lifetime Extension of Materials.

Li, L., Strachan, D. M., Davis, L. L., Li, H., & Qian, M. (1998). Gadolinium solubility limits in sodium-alumino-borosilicate glasses. In Scientific Basis for Nuclear Waste Management XXII, Materials Research Society. Pittsburgh, PA.

Strachan, D. M. (1999, Nov. 13). Mineralogy: Applications to nuclear waste disposal. Plenary presentation at the Twentieth Annual New Mexico Mineral Symposium, New Mexico Institute of Mining and Technology. Socorro, NM.

Wang, S. X., Wang, L. M., & Ewing, R. C. (1999). Electron irradiation of zeolites. In Zinkle, S. J., Lucas, G. E., Ewing, R. C., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Symposium Proceedings of the Materials Research Society, 540,361-366.

Project: 60392

Title: Radiolytic and Thermal Process Relevant to Dry Storage of Spent Nuclear Fuels

PI: Dr. Steven C. Marschman *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Petrik, N. G., Alexandrov, A. B., Vall, A., & Orlando, T. M. (1999, in press). Gamma radiolysis of water on oxide surfaces: Parameters controlling the energy transfer.

Petrik, N. G., Taylor, D. P., & Orlando, T. M. (1999). Laser-stimulated luminescence of yttria-stabilized cubic-zirconia crystals. J. Appl. Phys. 85,6770.

Simpson, W. C., Wang, W. K., Yarmoff, J. A., & Orlando, T. M. (1999). Photon- and electron-stimulated desorption of O + from zirconia. Surf. Sci., 423,225.

Publication Type: Presentation

Haustein, P. (1999, Aug. 22-26). Nuclear stimulated desorption at the surfaces of model SNF materials: Experiment and computer simulation. Invited presentation at the Annual Symposium on First Accomplishments of the Environmental Management Science Program, American Chemical Society. New Orleans, LA.

Hedhili, M. N., Yakshinskiy, B. V., & Madey, T. E. (1999, Mar. 21-25). Interaction of water with UO2 (001). National American Physical Society Meeting. Atlanta, GA.

Hedhili, M. N., Yakshinskiy, B. V., Madey, T. E., Dobrozemsky, R., & Yarmoff, J. (1999, Aug. 22-26). Interaction of water with uranium oxide surfaces. Annual Symposium on First Accomplishments of the Environmental Management Science Program. American Chemical Society. New Orleans, LA.

Orlando, T. M. (1999, Mar. 21-25). Quantum-resolved studies of condensed phase reactions. Invited presentation at the Annual Meeting of the Symposium on Free radicals in the Condensed Phase. American Chemical Society. Anaheim, CA.

Orlando, T. M., Petrik, N. G., Alexandrov, A. B., & Simpson, W. C. (1999, Feb. 24). Nonthermal processes on oxide surfaces and interfaces. Invited presentation at the Los Alamos National Laboratory. Los Alamos, NM.

Orlando, T. M., Petrik, N. G., Alexandrov, A. B., & Simpson, W. C. (1999, Feb. 26). Nonthermal processes on oxide surfaces and interfaces. Invited presentation at the Department of Chemistry, University of Utah. Salt Lake City, UT.

Orlando, T. M., Petrik, N. G., Alexandrov, A. B., & Simpson, W. C. (1999, Feb. 24-25). Nonthermal processes on oxide surfaces and interfaces. DOE Laboratory Catalysis Research Symposium. Albuquerque, NM.

Orlando, T. M., Petrik, N., Marshman, S., & Camaioni, D. M. (1999, Nov. 14-18). Nonthermal surface processes in the generation of gas in mixed wastes. Invited presentation at the Annual Meeting of the American Nuclear Society. Long Beach, CA.

Petrik, N., Marshman, S., Camaioni, D. M., & Orlando, T. M. (1999, Aug. 22-26). Nonthermal surface and interface processes in the storage of spent nuclear fuel and mixed wastes. Annual Symposium on First Accomplishments of the Environmental Management Science Program. American Chemical Society. New

Orleans, LA.

Project: 60451

Title: Mechanics of Bubbles in Sludges and Slurries
PI: Dr. Phillip A. Gauglitz *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Kam, S. I. & Rossen, W. R. (1999, in press). Anomalous capillary pressure, stress and stability of solids-coated bubbles. J. Colloid Interface Sci.

Publication Type: Presentation

Gauglitz, P. A., et. al. (1998, Jun.). Mechanics of bubbles in sludges and slurries: Initial progress. Hanford Technical Exchange. Richland, WA.

Gauglitz, P. A., et. al. (1999, Jan.). Mechanics of bubbles in sludges and slurries. Presented at the Hanford Site Technology Coordinating Group - Tank Subgroup. Richland, WA.

Gauglitz, P. A., Terrones, G., Aardahl, C. L., Mendoza, D. P., & Mahoney, L. A. (1999, Mar. 14-19). Mechanics of bubbles in sludges and slurries: Experimental studies and solid mechanics modeling results. Engineering Founda-tion Conference on Rheology in the Minerals Industry II. Oahu, HI.

Publication Type: Report

Kam, S. I. (1998). Interactions between bubbles and solids: Three applications. Department of Petroleum and Geosystems Engineering. The University of Texas, Austin, TX.

Project: 60474

Title: Ultrahigh Sensitivity Heavy Noble Gas Detectors for Long-Term Monitoring and Monitoring Air
PI: Dr. John D. Valentine *Institution:* Georgia Institute of Technology

Publication Type: Journal

Valentine, J. D. (1999). Evaluating detectors and pulse processing techniques. IEEE Transactions in Nuclear Science, 46(3).

Publication Type: Other

Valentine, J. D. (1999). Small prototype fluid transfer system and its performance. Nuclear Instruments and Methods in Physics Research, Section A, 422,820-825.

Project: 64907

Title: "Green" Biopolymers for Improved Decontamination of Metals from Surfaces: Sorptive Characterization and Costing Properties

PI: Dr. Brian H. Davison *Institution:* Oak Ridge National Laboratory

Publication Type: Poster

Davison, B. H. (1998, Nov. 17-18). Green biopolymers for decontamination. Poster presentation at Workshop on integration of end user needs with research projects for EMSP: Focus on Deactivation and Decommissioning at Savannah River Site.

Publication Type: Presentation

Davison, B. H. (1999, Sept. 12-17). Green biopolymer for decon of contaminated surfaces. Decontamination, Demolition, and Restoration (DD&R) Topical Meeting on Site Restoration of Government and Commercial Facilities. Knoxville, TN.

Project: 64946

Title: Mechanisms of Radionuclide-Hydroxycarboxylic Acid Interactions for Decontamination of Metallic Surfaces

PI: Dr. A.J. Francis *Institution:* Brookhaven National Laboratory

Publication Type: Presentation

Halada, G. P., et. al. (1999, May 2-6). Interaction of uranium with corrosion products formed on plain carbon steel. Paper presentation at the 195th Meeting of the Electrochemical Society. Seattle, WA.

Publication Type: Proceeding

Francis, A. J., Dodge, C. J., Gillow, J. B., Halada, G. B., & Clayton, C. R. (1999, Aug. 22-26). Decontamination of uranium contaminated metallic surfaces with uranium recovery. Paper presentation NUCL-65 at the Symposium on First Accomplishments of Environmental Management Science Program, 218th Annual Meeting of the American Chemical Society. New Orleans, LA.

Halada, G. P., et. al. (1999, Aug. 22-26). A spectroscopic study of the association of contaminant uranium with mild steel corrosion products. Paper presentation NUCL-61at the Symposium on First Accomplishments of Environmental Management Science Program, 218th Annual Meeting of the American Chemical Society. New Orleans, LA.

Project: 64965

Title: Supercritical Carbon Dioxide-Soluble Ligands for Extracting Actinide Metal Ions from Porous Solids

PI: Dr. Mark D. Dietz *Institution:* Argonne National Laboratory

Publication Type: Poster

Herlinger, A. W., Griffith, J. A., McAlister, D. R., & Barrans Jr., R. E. (1999, Aug. 22-26). Functionalized diphosphonic acid ligands for metal ion coordination in supercritical carbon dioxide. Poster presentation #33 at the First Accomplishments of the Environmental Management Sciences Program Symposium sponsored by the Division of Nuclear Chemistry and Technology at the 218th National A.C.S. Meeting. New Orleans, LA.

Project: 64979

Title: Decontamination and Decommissioning of PCB Sites at DOE: Extraction, Electrokinetics, and Hydrothermal Oxidation

PI: Dr. Edward A. Hamilton *Institution:* SCUREF

Publication Type: Poster

Pickett, J., et. al. (1998, Nov. 17-18). Decontamination & decommissioning of PCB sites at SRS. Poster presentation at the Workshop on Integration of End User Needs with Research Projects for the Environmental Management Science Program. Savannah River Site. Aiken, SC.

Publication Type: Presentation

Bruce, D. (1998, Nov. 15-20). Sonochemical oxidation of organic contaminants in waste water. Presentation at the AIChE Annual Meeting. Miami Beach, FL.

Matthews, M. (1998, Nov. 15-20). Mass transfer in CO2/surfactant systems. Presentation at the 1998 AIChE Annual Meeting. Miami Beach, FL.

Project: 65001

Title: Development of Novel, Simple Multianalyte Sensors for Remote Environmental Analysis

PI: Dr. Sanford A. Asher *Institution:* University of Pittsburgh

Publication Type: Journal

Holtz, J. H. & Asher, S. A. (1997). Intelligent polymerized crystalline colloidal array hydrogel film chemical sensing materials. Nature, 389,829-832.

Holtz, J. H., Holtz, J. S. W., Munro, C. H., & Asher, S. A. (1998). Intelligent polymerized crystalline colloidal arrays: Novel chemical sensor materials. Anal. Chem., 70,780-791.

Holtz, J., Weissman, J., Pan, G., & Asher, S. A. (1998). Mesoscopically periodic photonic crystal materials for linear and nonlinear optics and chemical sensing. Material Research Soc., 23,44-50.

Project: 65004

Title: Real-Time Identification and Characterization of Asbestos and Concrete Materials with Radioactive Contamination

PI: Dr. George Xu *Institution:* Rensselaer Polytechnic Institute

Publication Type: Journal

Naessens, E. P. & Xu, X. G. (1999). A non-destructive method to determine the depth of radionuclides in materials in-situ. Health Physics, 77(1),76-88.

Publication Type: Presentation

Chen, Q., Jiang, Z., Sun, F. G., & Zhang, X. -C. (1999, May). Two-fold improvement of THz optoelectronic generation and detection. CLEO'99. Baltimore, MD.

Jiang, Z., Sun, F. G., Chen, Q., & Zhang, X. -C. (1999, May). Electro-optic sampling near zero optical transmission point. CLEO'99. Baltimore, MD.

Project: 65352

Title: Developing a Fundamental Basis for the Characterization, Separation, and Disposal of Plutonium and Other Actinides in High Level Radioactive Waste: The Effect of Temperature and Electrolyte Concentrations on Actinide Speciation

PI: Dr. Sue B. Clark *Institution:* Washington State University

Publication Type: Journal

Clark, S. B. (1999, in press). The aqueous geochemistry of the rare earth elements. IX. A potentiometric study of Nd 3+ complexation with acetate in 0.1 molal NaCl solutions from 25-225° C. Geochim. Cosmochim. Acta.

Publication Type: Paper

Wood, S. A., Palmer, D. A., Wesolowski, D. J. (1999, Aug. 22-27). Determination of the solubility of crystalline Nd(OH)3 in sodium triflate solutions from 30 to 250 C with in situ pH measurement. Determination of the solubility of crystalline Nd(OH)3 in sodium triflate solutions from 30 to 250 C with in situ pH measurement. Ninth Annual V.M. Goldschmidt Conference Abstracts. Harvard University, Cambridge, MA. Lunar and Planetary Institute Contribution No. 791. Houston, TX. 329-330.

Project: 65366

Title: Physical, Chemical and Structural Evolution of Zeolite-Containing Waste Forms Produced From Metakaolinite and Calcined HLW

PI: Dr. Michael Grutzeck *Institution:* Pennsylvania State University

Publication Type: Proceeding

Siemer, D. D., Grutzeck, M. W., & Scheetz, B. E. (1999, Apr. 25-28). Comparison of materials for making hydroceramic waste forms. Proc. Amer. Ceram. Soc. Symposium on Waste Management Science and Technology in the Ceramic and Nuclear Industries, Indianapolis, IN. American Ceramic Society. Westerville, OH.

Project: 65370

Title: Actinide-Specific Interfacial Chemistry of Monolayer Coated Mesoporous Ceramics

PI: Dr. Glen E. Fryxell *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Fend, X., et. al. (1999). Self-assembled monolayers on mesoporous silica, a super sponge for actinides. In Mara, J. C. & Chandler, G. T. (Eds.), Ceramic Transactions, 93, Environmental Issues and Waste Management Technologies IV, 35-42.

Feng, X., et. al. (1999, in press). Self-assembled monolayers on mesoporous silica, a super sponge for actinides. Ceramic Transactions.

Fryxell, G. E., et. al. (1999, in press). Design and synthesis of selective mesoporous anion traps. Chemistry of Materials.

Publication Type: Other

Fryxell, G. E. & Liu, J. (1999, in press). Designing surface chemistry in mesoporous silica. In Papirer, E. (Ed.), Adsorption at Silica Surfaces. Marcel Dekker.

Publication Type: Presentation

Fryxell, G. E., et al. (1999, Jun.). Self-assembled monolayers on mesoporous supports: Synthesis of nanoscale hybrid materials and their applications. Presentation at the Northwestern Regional Meeting of the American Ceramic Society. Portland, OR.

Fryxell, G. E., et. al. (1999, Apr.). Design and synthesis of mesoporous lanthanide sorbent materials. Invited presentation at the 101st National Meeting of the American Ceramic Society.

Fryxell, G. E., et. al. (1999, Apr.). Environmental applications of interfacially modified mesoporous ceramics. Invited presentation at the 101st National Meeting of the American Ceramic Society.

Fryxell, G. E., et. al. (1999, Aug.). Environmental applications of Self-Assembled Monolayers on Mesoporous Supports (SAMMS). Invited presentation at the National Meeting of the American Ceramic Society. New Orleans, LA.

Fryxell, G. E., et. al. (1999, Jun.). High efficiency environmental sorbent materials: Self-assembled Monolayers on Mesoporous Support (SAMMS) for metal removal from aqueous systems. Presentation at the Symposium on Environmental Chemistry at the Northwestern Regional Meeting of the American Chemical Society. Portland, OR.

Fryxell, G. E., et. al. (1999, Jun.). High efficiency environmental sorbent materials: Self-assembled Monolayers on Mesoporous Supports (SAMMS) for metal removal from aqueous systems. Presentation at the Northwestern Regional Meeting of the American Ceramic Society. Portland, OR.

Fryxell, G. E., et. al. (1999, Jun.). Self assembled monolayers on mesoporour supports: Synthesis of nanoscale hybrid materials and their applications. Presentation at the Symposium on Nanoscale Materials at the Northwestern Regional Meeting of the American Chemical Society. Portland, OR.

Publication Type: Press release

Fryxell, G. E. (1999, Apr. 11). PNNL focuses on healthy environment. Tri-City Herald, D1.

Fryxell, G. E. (1999, Mar.). Metal eaters. Popular Science, 34.

Project: 65371

Title: Numerical Modeling of Mixing of Chemically Reacting, Non-Newtonian Slurry for Tank Waste Retrieval

PI: Dr. David A. Yuen *Institution:* University of Minnesota

Publication Type: Journal

Ten, A. A., Podladchikov, Y. Y., Yuen, D. A., Larsen, T. B., & Malevsky, A. V. (1998). Comparison of mixing properties in convection with the particle-line method. Geophys. Res. Lett., 25(16),3205-3208.

Ten, A. A., Yuen, D. A. & Podladchikov, Y. Y. (1999, in press). Numerical modeling of mixing of chemically reacting, non-Newtonian slurry for tank waste retrieval. Electronic Geosciences.

Publication Type: Presentation

Onishi, Y., Trent, D. S., Michener, T. E., Van Beek, J. E., & Rieck, C. A. (1999, Jul. 18-23). Simulation of radioactive tank waste mixing with chemical reactions. FEDSM99-7786, presentation at the 3rd ASME/JSME Joint Fluids Engineering Conference. San Francisco, CA.

Publication Type: Proceeding

Onishi, Y. & Trent, D. S. (1999). Mobilization modeling of erosion-resisting radioactive tank waste. Proceedings of the Rheology in the Mineral Industry II. United Engineering Foundation, New York, NY. 45-56.

Onishi, Y. & Trent, D. S. (1999, Mar. 14-19). Mobilization modeling of erosion-resisting radioactive tank waste. Proceedings of the Rheology in the Mineral Industry II, Kahuku, Oahu, HI. Organized by United Engineering Foundation. New York, NY. 45-56.

Onishi, Y., Trent, D. S., Michener, T. E., Van Beek, J. E., & Rieck, C. A. (1999, Jul. 18-23). Simulation of radioactive tank waste mixing with chemical reactions. FEDSM99-7786: Proceedings of 3rd ASME/JSME Joint Fluids Engineering Conference. San Francisco, CA.

Project: 65408

Title: Mechanisms and Kinetics of Organic Aging in High-Level Nuclear Wastes
PI: Dr. Donald M. Camaioni *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Autrey, S. T. (1999, Apr. 30). Nitrosyl transfer reactions are not catalyzed by Al(OH)4. Notre Dame Radiation Laboratory and Pacific Northwest National Laboratory EEMSP Coordination Meeting and Technical exchange. Notre Dame, IN.

Camaioni, D. M. (1998, Nov. 17). Mechanisms and kinetics of organic aging in high level wastes. EMSP/Tanks Focus Area Workshop. Richland, WA.

Camaioni, D. M. (1998, Oct. 29). Mechanisms and kinetics of the degradation of organic complexants in nuclear waste. Chemistry Seminar, Notre Dame Radiation Laboratory. Notre Dame, IN.

Camaioni, D. M. (1999, Aug. 22-26). Thermochemical kinetic analysis of thermal pathways for oxidation of organic complexants in high level wastes. First Accomplishments of the Environmental Management Science Program. Annual Meeting of the American Chemical Society. New Orleans, LA.

Project: 65410

Title: Rapid Migration of Radionuclides Leaked from High-Level Waste Tanks: A Study of Salinity Gradients, Wetted Path Geometry and Water Vapor Transport
PI: Dr. Anderson L. Ward *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Selker, J. S. (1998, Dec. 5-10). Fingered flow from high salinity sources. Presented at the AGU Fall Meetings. San Francisco, CA.

Ward, A. L. & Gee, G. W. (1999, Oct. 31 - Nov. 4). A numerical analysis of wetting front instability induced by infiltration of highly saline fluids. Symposium on Preferential Flow, Soil Science Society of America Annual Meeting. Salt Lake City, UT.

Project: 65421

Title: Correlation of Chemisorption and Electronic Effects for Metal/Oxide Interfaces: Transducing Principles for Temperature-Programmed Gas Microsensors

PI: Dr. Stephen Semancik *Institution:* National Institute of Standards & Technology - Boulder

Publication Type: Presentation

Cavicchi, R. E. (1998, Nov. 17). Correlation of chemisorption and electronic effects for metal/oxide interfaces: Transducing principles for temperature programmed gas microsensors. Environmental Management Science Program - Tank Focus Area Workshop. Richland, WA.

Cavicchi, R. E. (1999, Sept. 17-22). Microhotplate gas sensor arrays. Presentation at the SPIE International Symposium on Environmental and Industrial Sensing. Boston, MA.

Ding, J. (1999, Sept. 17-22). Quantification of a single component gas in air with a microhotplate gas sensor using partial least squares techniques. Presentation at the SPIE International Symposium on Industrial and Environmental Sensing. Boston, MA.

McAvoy, T. J. (1999, Aug. 24). Modeling microhotplate gas sensors. Presentation at the ACS National Meeting. New Orleans, LA.

Panchapakesan, B. (1999, Apr. 7). Micromachined array studies of tin oxide films: Nucleation, structure and gas sensing characteristics. MRS Spring National Meeting. San Francisco, CA.

Semancik, S. (1999, Aug. 24). Microarrays as platforms for gas microsensor development and efficient materials research. Presentation at the ACS National Meeting. New Orleans, LA.

Semancik, S. (1999, Sept.). Solid state gas microsensors for environmental and industrial monitoring. Presentation at the SPIE International Symposium on Industrial and Environmental Sensing. Boston, MA.

Walton, R. M. (1999, Jun. 7). Processing methods for selected area film deposition and preparation on microsensor platforms using thermal and potential control. 10th International Conference on Solid-State Sensors and Actuators. Sendai, Japan.

Publication Type: Proceeding

Panchapakesan, B., DeVoe, D. L., Cavicchi, R. E., Walton, R. M., & Semancik, S. (1999, in press). Micromachined array studies of tin oxide films: Nucleation, structure and gas sensing characteristics. Proceedings of the MRS, Spring 1999.

Walton, R., et. al. (1999, Jun.). Processing methods for selected area film deposition and preparation on microsensor platforms using thermal and potential control. Digest 10th International Conference on Solid-State Sensors and Actuators, 1,676-679. Sendai, Japan.

Project: 65422

Title: Modeling of Spinel Settling in Waste Glass Melter
PI: Dr. Pavel Hrma *Institution:* Pacific Northwest National Laboratory

Publication Type: Paper

Hrma, P. (1999). Spinel precipitation in high-level waste glass. Proceedings of the 5th ESG Conference. Prague, Czechoslovakia.

Project: 65425

Title: Mass Spectrometric Fingerprinting of Tank Waste Using Tunable, Ultrafast Infrared Lasers
PI: Dr. Richard F. Haglund *Institution:* Vanderbilt University

Publication Type: Presentation

R. F. Haglund, Jr., (1999, Jun.). The future of tunable, ultrafast lasers in materials analysis and processing. Plenary lecture at the American Society for Mass Spectrometry. Dallas, TX.

Research Transfers

EMSP RESEARCH TRANSFER

The EMSP provides research resources and results that are intended, in part, to "bridge the gap" between broad fundamental research that has wide-ranging applications such as that performed in the Department's Office of Science, and needs driven applied technology development that is conducted in Environmental Management's Office of Science and Technology. In support of this, the focused research performed in the EMSP is intended to be transferred for utilization by other programs within DOE or to end-users outside the Department.

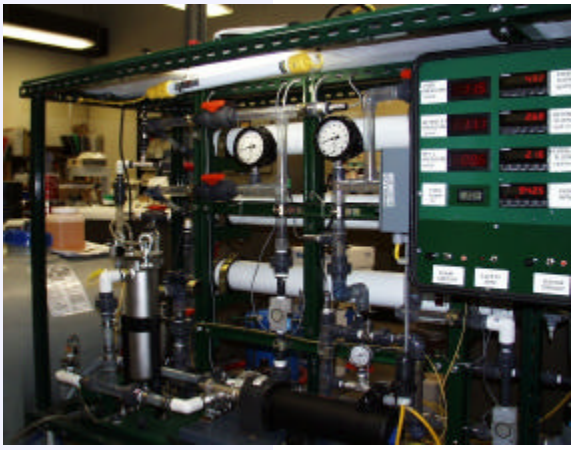
As research within the EMSP matures, the results from this research should support development of new and innovative ways to reduce risk and cost within EM. In part, the research should address the early, focused research stage of the technology development/deployment cycle for development of new technologies to address cleanup problems within EM. Part of the focus of the EMSP is to integrate the program's research with EM Focus Areas, DOE sites and commercial interests to support technology development. While much of the research is not yet at a stage of maturity to transfer, many successes have been reported. To date, the reported accomplishments include transfers to:

- Commercializations 6
- Field Tests 6
- Focus Areas & Cross Cuts (Deployed or Demonstrated) 3
- Patents 8
- Processes - IPP 1
- Products - Unknown 1

Project: 54674

Title: Design and Development of a New Hybrid Spectroelectrochemical Sensor
PI: Dr. William R. Heineman *Institution:* University of Cincinnati

Description: A proposed new sensor concept proposed combines the elements of electrochemistry, spectroscopy and selective partitioning into a single device that provides three levels of selectivity. This type of sensor has many potential applications at DOE sites. As an example, the enhanced specificity embodied in this new sensor design is well-suited to the analytical problem posed by the addition of ferrocyanide to radioactive tank wastes at the USDOE Hanford Site. A demonstration of a sensor package (mircocell and Instrumentation) in was performed on waste tank sample.
Transfer Type: Field Test *Transfer Date:*
Contact: Dr. Heineman - University of Cincinnati
Transferring Organization: Hanford Site



Ultrafiltration unit used in field demonstration for removal of radioactive cations and anions. [see Project #54724]

Project: 54724

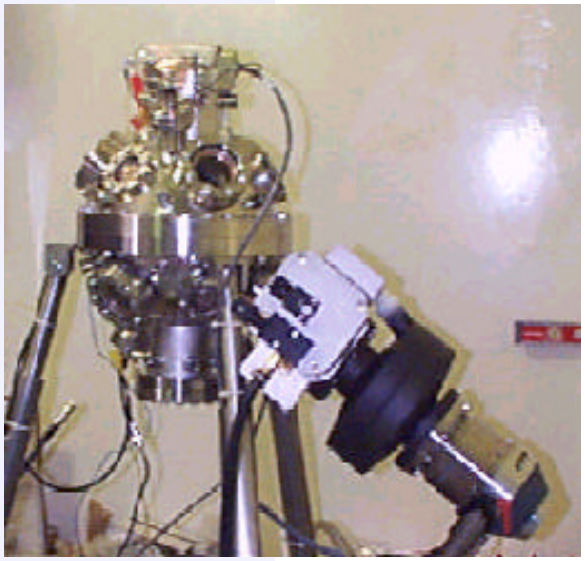
Title: Synthesis of New Water-Soluble Metal-Binding Polymers: Combinatorial Chemistry Approach
PI: Dr. Barbara F. Smith
Institution: Los Alamos National Laboratory

Description: Polymer Filtration (PF), which uses water-soluble metal-binding polymers to sequester metal ions in dilute solution with ultrafiltration (UF) to separate the polymers, is a new technology to selectively remove or recover hazardous and valuable metal ions. We have focused on four areas including the development of: (1) synthetic procedures, (2) small ultrafiltration equipment compatible with organic-and aqueous-based combinatorial synthesis, (3) rapid assay techniques, and (4) polymer characterization techniques.We have entered into partnership to use Polymer Filtration in Electroplating industry.

Transfer Type: Commercialization - Product *Transfer Date:*
Contact: NA
Transferring Organization: NA

Project: 54751

Title: High Fluence Neutron Source for Nondestructive Characterization of Nuclear Waste
PI: Dr. Mark M. Pickrell *Institution:* Los Alamos National Laboratory



Two commercial partners have applied for a license for the High Fluence Neutron Source, shown here in the laboratory. [see Project #54751]

Description: We are addressing the need to measure nuclear wastes, residues, and spent fuel in order to process these for final disposition. One of the primary methods for waste assay is by active neutron interrogation. We plan to improve the capability of all active neutron systems by providing a higher intensity neutron source (by about a factor of 1,000) for essentially the same cost, power, and space requirements as existing systems. We have received 2 request from commercial vendors to commercialize this technology once available.

Transfer Type: Commercial
Transfer Date:
Contact: Manfred Frey, Michael Hurwitz
Transferring Organization: MF Physics, Inc., Gamma Metrics, Inc.

Project: 54837

Title: Phytoremediation of Ionic and Methyl Mercury Pollution
PI: Dr. Richard B. Meagher *Institution:* University of Georgia

Description: Our long-term goal is to enable highly productive plant species to extract, resist, detoxify, and/or sequester toxic heavy metal pollutants as an environmentally friendly alternative to physical remediation methods. We have focused this phytoremediation research on soil and water-borne ionic and methylmercury. We engineered several plant species (e.g., Arabidopsis, tobacco, canola, yellow poplar, rice) to express the bacterial genes, merB and/or merA, under the control of plant regulatory sequences. These transgenic plants acquired remarkable properties for mercury remediation. Our project has been so successful that a private company, PhytoWork Inc. has been created.
Transfer Type: Commercial *Transfer Date:* December 1, 1998
Contact: Richard Meagher
Transferring Organization: PhytoWork Inc.

Project: 54973

Title: A Novel Energy-Efficient Plasma Chemical Process for the Destruction of Volatile Toxic
PI: Dr. Lal A. Pinnaduwage *Institution:* Oak Ridge National Laboratory

Description: Patent - "Destruction of Low-concentrations of Volatile Toxic Compounds using glow discharge"
Transfer Type: Patent *Transfer Date:*
Contact: Dr. Lal A. Pinnaduwage
Transferring Organization: Oak Ridge National Laboratory

Description: Patent - "A Plasma Mixing Method and Device for Plasma Processing of Materials"
Transfer Type: Patent *Transfer Date:*
Contact: Dr. Lal A. Pinnaduwage
Transferring Organization: Oak Ridge National Laboratory

Description: Patent - "Method for Suppression of dust formation in Material Processing Discharges"
Transfer Type: Patent *Transfer Date:*
Contact: Dr. Lal A. Pinnaduwage
Transferring Organization: Oak Ridge National Laboratory

Project: 55087

Title: Design and Synthesis of the Next Generation of Crown Ethers for Waste Separations: An Inter-Laboratory Comprehensive Proposal
PI: Dr. Bruce A. Moyer *Institution:* Oak Ridge National Laboratory

Description: Owing to the high levels of radiation and heat generated by the fission-product Cs-137, efficient cesium separation from high-level wastes (HLWs) has been elevated to extreme importance at Hanford, the

Savannah River Site (SRS), and Idaho Falls, where multi-billion dollar projects will carry out this and other HLW separations. Referred to as Alkaline-Side CSEX (Cesium Solvent Extraction), the ORNL invention (U.S. Pat. Appl. 60/057,974, September 3, 1998) provides the first practical application of calixarene-crown extractants to treatment of HLWs by solvent extraction. An effective form of the extractant was first synthesized at ORNL and recently transferred to the commercial sector. Batch tests on actual HLW by collaborators at both Hanford and the SRS in the past year have confirmed the effectiveness of the ORNL process, and a 24-stage centrifugal-contactor demonstration at Argonne National Laboratory proved economic viability. Results from the batch and engineering tests showed that stringent requirements of a 40,000-fold reduction in Cs-137 activity in the waste and a 12-fold concentration can be readily met. In addition to meeting these SRS decontamination and concentration needs, key advantages of the ORNL process include the following: (1) The process does not require adjustment of the waste feed stream. (2) Extraction is very selective. (3) Scrubbing and stripping of the solvent can be accomplished with very dilute acidic solutions. (4) The process is compact and involves liquid streams. These advantages reduce costs by minimizing consumption of chemicals, secondary waste production, volume of vitrified waste form, and plant space. The cesium-concentrated stream produced by the process is expected to be so pure that it will require negligible downstream processing and will have negligible impact on the volume of the final vitrified waste form, which is costly to produce and store.

Transfer Type: Commercial *Transfer Date:*
Contact:
Transferring Organization: IBC Advanced Technologies

Description: Patent – Alkaline-Side CSEX (Cesium Solvent Extraction), U.S. Pat. Appl. 60/057,974, September 3, 1998
Transfer Type: Patent *Transfer Date:*
Contact: Bruce Moyer
Transferring Organization: Oak Ridge National Laboratory

Description: The role of the EMSP project in my lab entailed performing a fundamental investigation of the mechanism of cesium extraction so as to understand the nature of the complexes formed between the cesium ion and the extractant molecule. This fundamental information played a crucial role in the successful process development under ESP funding. Indeed, without the fundamental information providing the needed insight at just the right time, the process development would have failed to advance fast enough to meet the emergency need to test new technology at the SRS.
Transfer Type: Focus Area -Process *Transfer Date:*
Contact: Bruce Moyer
Transferring Organization: Oak Ridge National Laboratory

Project: 55264

Title: High Resolution Definition of Subsurface Heterogeneity for Understanding the Biodynamics of Natural Field Systems: Advancing the Ability for Scaling to Field Conditions

PI: Dr. Ernest L. Majer *Institution:* Lawrence Berkeley National Laboratory

Description: We have been using our technology at the TAN site at INEEL to aid in defining the plume movement and location.

Transfer Type: Field Test *Transfer Date:*

Contact: Tom Woods and John Bukowski

Transferring Organization: Parsons

Project: 55328

Title: Novel Analytical Techniques Based on an Enhanced Electron Attachment Process

PI: Dr. Lal A. Pinnaduwage *Institution:* University of Tennessee at Knoxville

Description: The objective of our research program is to develop novel analytical techniques that can be expected to be applicable for a wide variety of molecules with high sensitivity. These are based on the recently discovered enhanced negative ion formation process involving electron attachment to highly-Rydberg states of molecules. We are using two approaches to produce the precursor highly-excited states; one is laser excitation, and the other is discharge based. A patent, "A Novel Glow Discharge Process for Analytical Applications," Patent No. 5,896,196 was issued for these analytical techniques.

Transfer Type: Patent *Transfer Date:* April 1, 1999

Contact: PI

Transferring Organization: University of Pennsylvania

Project: 55416

Title: Control of Biologically Active Degradation Zones by Vertical Heterogeneity: Applications in Fractured Media

PI: Dr. Frederick S. Colwell

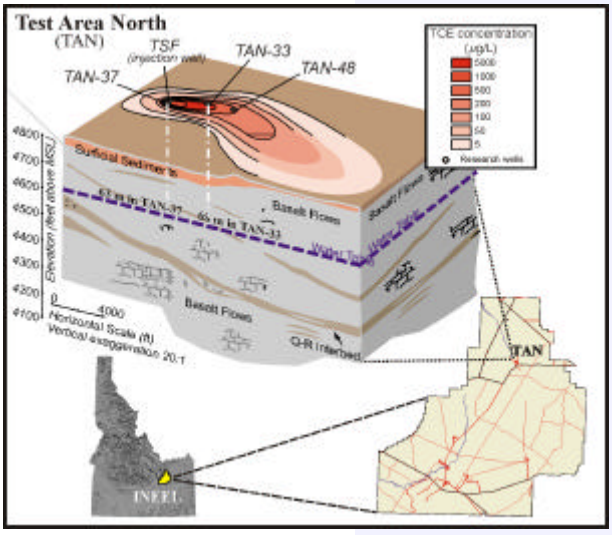
Institution: Idaho National Engineering and Environmental Laboratory

Description: Coring, well completion of TAN-48 (INEEL), Design, implementation of Flexible Liner Underground Technology, and Characterization of effect of lactate-induced bioremediation.

Transfer Type: Field Test *Transfer Date:* 12/1/98

Contact: Lance Peterson, Kent Sorenson, and Joe Rothermel

Transferring Organization: Idaho National Engineering and Environmental Laboratory; Parsons



Microorganisms with the capability of degrading dissolved TCE in the fractured basalts beneath the INEEL Test Area North are being studied to determine their vertical distribution and to assess how geohydrological factors associated with this complex subsurface environment control their activities. [see Project #55416]

Project: 60115

Title: Advanced High Resolution Seismic Imaging, Material Properties Estimation and Full Wavefield Inversion for the Shallow Subsurface

PI: Dr. Alan Levander *Institution:* Rice University

Description: Conducted a high resolution seismic profile for subsurface characterization at a DNAPL site at a DOD facility in August of last year. Currently processing the data and are planning to return to the site for additional work.

Transfer Type: Field Test *Transfer Date:*

Contact:

Transferring Organization:

Project: 60158

Title: Development of Radon-222 as a Natural Tracer for Monitoring the Remediation of NAPL Contamination in the Subsurface

PI: Dr. Lewis Semprini *Institution:* Oregon State University

Description: We have conducted Radon-222 and Surveys at Site-300 at the Lawrence Livermore National Laboratory. This site is highly contaminated with TCE. The radon results were encouraging, and indicated a zone of NAPL likely existed.

Transfer Type: Field Test *Transfer Date:*

Contact: Rolf Halden (925-422-0655 or halden1@llnl.gov)

Transferring Organization: Lawrence Livermore National Laboratory

Project: 60162

Title: Enhancements to & Characterization of the Very Early Time Electromagnetic (VETEM) Prototype Instrument & Applications to Shallow Subsurface Imaging at Sites in the DOE Complex

PI: Dr. David L. Wright *I* *nstitution:* U.S. Geological Survey - Denver

Description: The VETEM prototype system has been to INEEL twice since the beginning of our EMSP funding. The first trip was in July, 1998 for a demonstration at the Cold Test Pit. The second trip was in Nov-Dec of 1998 to do a survey of Pit 9.

Transfer Type: Field Test *Transfer Date:* July 1, 1999

Contact: Aran Armstrong & George Schneider

Transferring Organization:

Project: 60197

Title: Microsensors for In-site Chemical, Physical, and Radiological Characterization of Mixed Waste

PI: Dr. Thomas G. Thundat *Institution:* Oak Ridge National Laboratory

Description: The goal of this project is to develop a single-sensor platform approach that is based on the recently discovered extreme sensitivity of microcantilever sensing using adsorption-induced forces. The objective of this research is to gain better understanding of the basic mechanism of

adsorption-induced differential surface stress variation and to use this concept for developing sophisticated microsensors for chemical and radiological sensing in liquids. A patent "Electromagnetic and nuclear radiation detector using micromechanical sensors", T. Thundat, E.A. Wachter, and R.J. Warmack, ESID-1604-X-1 is currently pending.

Transfer Type: Patent *Transfer Date:*
Contact: Dr. Thomas Thundat
Transferring Organization: Oak Ridge National Laboratory

Project: 60231

Title: Novel Miniature Spectrometer for Remote Chemical Detection
PI: Dr. Andrew C. R. Pipino *Institution:* National Institute of Standards & Technology -

Description: Discussing deployment of miniature spectrometer at the Savannah River Site for groundwater monitoring.
Transfer Type: Focus Area -Product *Transfer Date:*
Contact: Michael G. Serrato
Transferring Organization: Savannah River

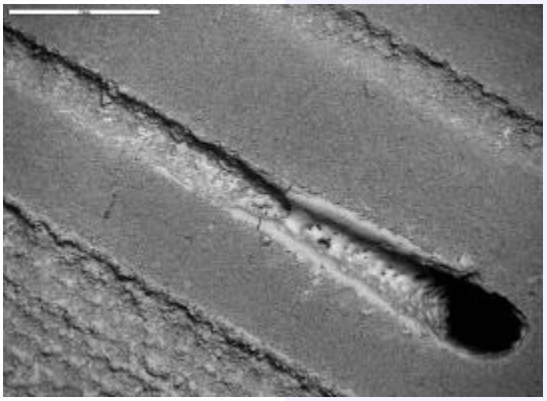
Description: A Cooperative Research and Development Agreement (CRADA) is being negotiated with to develop and build prototype, portable, miniature spectrometers, which will be fiber-optic-coupled to inexpensive diode laser sources.
Transfer Type: Commercial *Transfer Date:*
Contact:
Transferring Organization: Informed Diagnostics, Inc

Description: A entirely new class of chemical sensors is being developed that will enable qualitative and quantitative remote, real-time, optical diagnostics of chemical species in hazardous gas, liquid, and semi-solid phases through a completely novel implementation of cavity ring-down spectroscopy. Negotiations with a commercial partner are in progress.
Transfer Type: Product *Transfer Date:*
Contact:
Transferring Organization: Not disclosed at this time

Project: 60283

Title: Waste Volume Reduction Using Surface Characterization and Decontamination by Laser Ablation
PI: Dr. Michael J. Pellin
Institution: Argonne National Laboratory

Description: The objectives of this research are to determine the mechanism and efficacy of laser ablation in removing contaminated surface layers, to understand the chemistry of contaminated concrete surfaces, and to chemically and physically characterize the captured ablation effluent which



Cement surface following Laser Ablation. [see Project #60283]

would become the stored waste. While the focus of this project is on concrete, the technology should be applicable to any surface requiring removal. Efforts are underway to establish a CRADA with Zawtech Inc.

Transfer Type: Commercial *Transfer Date:*
Contact:
Transferring Organization: Zawtech Inc.

Project: 60363

Title: Optimization of Thermochemical, Kinetic, and Electrochemical Factors Governing Partitioning of Radionuclides during Melt Decontamination of Radioactively Contaminated Stainless Steel

PI: Dr. James A. Van Den Avyle *Institution:* Sandia National Laboratories

ElectroSlag Remelting (ESR) process for radioactive decontamination of stainless steel scrap for metal recycle. [see Project #60363]

Description: We have conducted a successful technology demonstration with the Russians at a site near Krasnoyarsk (K-26), where they electroslag remelted stainless steel reactor coolant piping that was contaminated with Pu and other radionuclides. The resulting metal ingot was fully analyzed and was clean enough to meet Russian criteria for outside reapplication (sale). We are working with them to obtain significant new funding to set up a full scale commercial melt decontamination facility there to recycle stainless steel. We are also paying for a few additional melts there to further characterize the process.

Transfer Type: Process *Transfer Date:*
Contact: James Van den Avyle
Transferring Organization: Sandia National Laboratory

Project: 64982

Title: Metal Ion Analysis Using Near-Infrared Dyes and the “Laboratory-on-a-Chip”

PI: Dr. Greg E. Collins *Institution:* Naval Research Laboratory

Description: This project addresses the need for developing a highly sensitive and selective, portable radionuclide analyzer which would permit a low-cost and timely characterization of DOE remediation sites. Through the application of near-infrared fluorophore tagged macrocycles, in combination with the capillary electrophoretic separation of radionuclide and heavy metal complexes on a microchip, we propose an innovative, low cost characterization approach to gaining timely characterization data in

the field. DDFA has committed to perform Large Scale Demonstration on the "Laboratory-on-a-Chip".

Transfer Type: Focus Area -Product *Transfer Date:*
Contact: Dick Meservey
Transferring Organization: DDFA

Project: 65004

Title: Real-Time Identification and Characterization of Asbestos and Concrete Materials with Radioactive Contamination

PI: Dr. George Xu *Institution:* Rensselaer Polytechnic Institute

Description: Patent – "Non-destructive In-situ Method and Apparatus for Determining Radionuclide Depth in Media" by X. George Xu and Edward P. Naessens. 6/11/1999. U.S. Patent Serial No. 09/333,660

Transfer Type: Patent *Transfer Date:* June 11, 1999
Contact: PI
Transferring Organization:

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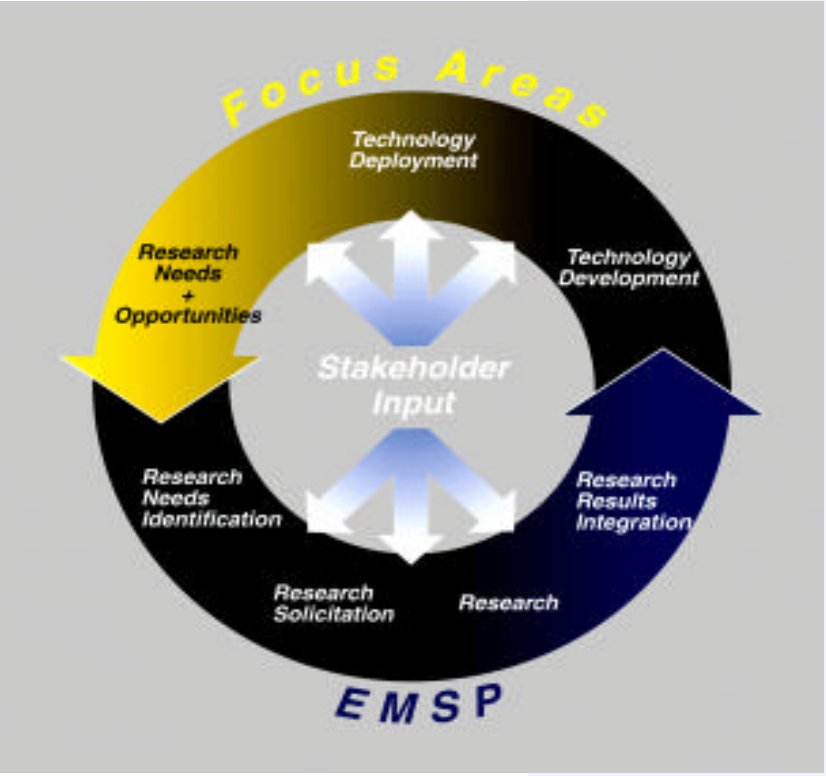
TOPICAL WORKSHOPS

Workshops and other interactive forums sponsored by the EM Science and Risk Policy Programs are useful research integration tools because they bring researchers and technology users together. EMSP workshops either center on subject-specific or site-specific topics, using a particular theme to highlight pressing problems within EM, or are held in conjunction with Focus Area reviews and professional society meetings. The objective of tying an EMSP workshop to a Focus Area review is to better define end-user needs so researchers fully understand the site problem for which their research is targeted. Workshops typically feature presentations of the research being conducted by the principal investigators, with industry and/or end-user participation and feedback.

Such forums allow the EMSP researchers to learn about and discuss actual technology needs with the end-users. At the same time, site representatives and other end-users have an opportunity to hear about science developments directly from those conducting the R&D work. The EM/OST Focus Areas provide the linkage between the EMSP projects and the Department's ongoing waste management and clean-up programs within the Offices of Waste Management (EM-30), Environmental Restoration (EM-40), and Nuclear Materials and Facility Stabilization (EM-60). The five Focus Areas OST currently supports are:

- Mixed Waste Focus Area (MWFA),
- Nuclear Materials Focus Area (NMFA),
- Subsurface Contaminants Focus Area (SCFA),
- Deactivation and Decommissioning Focus Area (DDFA),
- Tanks Focus Area (TFA).

Through communication and cooperation between EM's site end-users, the Focus Areas identify opportunities to integrate the research results of EMSP projects to improve performance and reliability of their baseline clean-up technologies. The Focus Areas also evaluate EMSP projects and results to reveal opportunities to develop breakthrough technologies to solve EM's long-term environmental problems and reduce risk. Figure 1 shows the circular flow of information between the EMSP and the Focus Areas.



The EMSP Process Relative to the Focus Areas

Moving research results to application by end-users involves:

- Working with DOE problem holders to identify needs and priorities
- Working with the OST Focus Areas to coordinate activities
- Communicating science results to Focus Area technology developers and EM problem holders.

Dialogue between the end-users and the researchers regarding how the research results can be applied enables sufficient customer understanding of the EMSP projects to "pull" technology down the chain from research to deployment. Focus Areas indicate and facilitate interaction where there is a potential application and provide recommendations for tailoring planned research activities towards Focus Area needs.

The workshops have been very successful and the presentations made by the researchers have been of consistently high quality. Details of the past and planned workshops, including presentations, are available on our program web page (http://emsp.em.doe.gov/workshops/index.htm).

Workshop on Integration of End-user needs with Research Projects for EMSP
July 9-10, 1998
Savannah River Site, SC

The purposes of this workshop were to inform EMSP principal investigators of environmental restoration program needs at SRS, to inform the end-users of currently funded EMSP projects that have relevance to SRS needs, and to determine and plan a program to meet gaps and unmet needs using EMSP research. Among the seventy-five representatives in attendance were EMSP principal investigators; STCG and SCFA end-users; scientists from regional universities, including minority serving institutions and university consortia; DOE contributors; and M&I contractors. The workshop participants received overviews of EMSP and SCFA technologies currently in use at SRS, as well as SRS end-user needs and STCG activities. Tours were available for workshop participants to see SRS needs first-hand.

Three subgroups were formed to develop deployment plans for (1) phytoremediation, (2) DNAPL, characterization, and bioremediation, and (3) metals and rads. The outcome of the phytoremediation subgroup was extremely successful in providing an abbreviated deployment project plan. It was concluded that phytoremediation was a viable technology to meet two stated needs: (1) deploy passive technology for attenuation of VOC, and (2) utilize innovative technologies to replace pump and treat technology. The subgroup proposed three phytoremediation pilot scale demonstrations utilizing loblolly pines, poplar trees, and an aquatic lagoon system. Timelines and cost estimates to process the projects from the science phase through deployment were developed. The DNAPL, characterization, and bioremediation subgroup was less optimistic about the application of the selected southeastern science projects to SRS needs. SRS has large DNAPL plumes where characterization is needed and improved off-gas treatment from vapor extraction technologies is desirable. These selected projects address a gap at SRS. The technologies are 5-9 years away from deployment and currently available technologies allow cleanup to progress. The metals and rads subgroup directed the participating PIs towards discussions with high level waste end-users.

INEEL Science Integration Workshop
October 20-22, 1998
Idaho Falls, Idaho

This site-specific workshop included 101 attendees with interests in four science areas: fractured rock, high level waste (calcine separations), decontamination and decommissioning (D&D), and LandTech. Fractured rock sessions included 12 presentations of ongoing research, followed by two working sessions to discuss opportunities for increased collaboration, as well as the identification of science and technology gaps related to understanding and remediating contaminated fractured rock environments. The D&D group toured the sewage treatment facility at CFA, Pit 9, and the nuclear airplane engine exhibit. The high level waste group toured the calcining facility at INTEC. The LandTech group developed a set of research requirements during their breakout session, and also toured Box Canyon.

Interactions between the PIs and end-users included the following:

- Application of "Lab on a Chip" where Brad Frazee (INEEL) and Greg Collins (Naval Research Laboratory) discussed needs characterization information concerning their important constituents. It was decided that (1) Tom Thiel would get information on the top twelve hitters of "Lab on a Chip" to Greg Collins; (2) Greg would contact the INEEL Sample Management Office in order to test the samples; (3) large scale demonstration of "Lab on a Chip" would be done by Greg and Dick Meservey; and (4) Greg would keep Dick apprised on further research done, with the goal to be using the "Lab on a chip" in the field as part of a large scale demonstration project.

- Mike Savina and Maurice Ross of TRA met with Zawtech, Inc. while in Idaho Falls and they are discussing CRADAs and other industrial partnerships regarding Laser Ablation and Robotics for scabbling.

- Information from INEEL requested transfer of knowledge regarding D&D cost estimates from Brad Frazee. Completed by providing the researchers with the URL that has the information on it.

- Brad Frazee and Dick Meservey will track progress of a novel class of sensors based on light diffraction utilizing polymerized colloidal crystalline arrays for longer-term usage (Sanford Asher). DDFA is interested in field testing a portable sensor.

- Inorganic Ion Exchange Materials for Environmental Restoration research is a promising area because there is an increasing concern regarding water treatment as the size of the reactor being decontaminated and decommissioned increases. The end-users believe there will be a need in the future as commercial power plants are decommissioned. Full-scale membrane filters are needed to cleanup fuel storage basins at the INEEL to warm waste pond disposal limits.

Workshop on Integration of End-user needs with Research Projects for EMSP Focus on Deactivation and Decommissioning November 17-18, 1998 Savannah River Site, SC

The purposes of the workshop were to:

- Increase the awareness of the EMSP principal investigators of the role of the DDFA and thereby increase the applicability of their projects to the D&D mission of DOE,
- Improve SRS knowledge of the EMSP research,
- Identify EMSP projects that have direct usefulness to SRS D&D activities, and
- Determine and discuss EMSP project needs.

Twenty principal investigators and 31 individuals representing the DDFA, end-users, scientists, and DOE program representatives listened to overviews of the EMSP program and the DDFA, discussed lessons learned from the D&D breakout session at the INEEL Workshop and results from the D&D Large Scale Demonstration at the INEEL, and toured SRS's D&D Large Scale Demonstration. The EMSP principal investigators provided a short overview of their projects and afterwards hosted a poster session.

The EMSP PIs gained an improved knowledge of the D&D needs of DOE as a result of the workshop. SRS and selected segments of the DOE complex were informed of the EMSP D&D related research. SRS will provide mentors to several of the projects. Fourteen PIs identified current needs to increase the effectiveness of their research projects. These needs include:

- Representative samples that can be used to test the decontamination process being developed in the laboratory. (A.J. Francis)

- Replicate contaminated metal coupon for quantitative lab tests on biological coatings for removal of contamination radiation. Need to know what is considered "fixed contamination". (Brian Davison)

- Monitoring of mixtures of radionuclides and examining actual samples (e.g. concrete drill samples). Field testing to compare to baseline technologies. (Greg Collins)

- Concrete surface samples and priority of contaminants on concrete (particularly radionuclides). (Brian Spalding)

- Indoor/outdoor location with radioactive airborne contamination to test sampling equipment. Identification of industrial partners. (Piotr Wasiolek)

- More information of the structure and composition of surface contaminants to enable design of more realistic experiments. (Steve Babayan)

- Composition of radioactively contaminated surface layers on pipes and storage tanks, (i.e., type of radionuclides, heavy metal ions, etc.), level of contamination, thickness of surface film. Need 2" x 2" samples. (Carlos Melendres)

- Information on general residues (organics/inorganics/particulates). (R.M. Counce)

- End-users that could benefit from: (1) predictive capability of diffusion between contaminants (plutonium, uranium, etc.) and metal they are in contact with/ contained by (e.g., glove box components and steel storage containers), and (2) a mobile apparatus to detect degree of contamination, chemical and physical characterization of contaminant that has been painted over as opposed to being in a steel container. (Bernard Cooper)

- Database of: (1) alloys/metals commonly contaminated, (2) atmospheric conditions of typical storage and operation in D&D facilities, (3) typical paints/surface coatings that are found on these surfaces, and (4) method and length of time of contamination or exposure to contaminants. (Gary Halada)

These needs range from common samples that could be decontaminated to a mini demonstration facility where representative radioactive samples could be decontaminated with prototype equipment to evaluate the prototype before proceeding to the large scale demonstration facilities provided by the DDFA. Many of the university PIs do not have licenses or facilities to handle radioactive materials, yet need access to these materials for their research.

Tanks Focus Area (TFA) Workshop
November 17-18, 1998
Richland, Washington

The Tanks Focus Area (TFA) develops technologies to safely and efficiently remediate radioactive waste stored in underground tanks at four sites nationwide. This work is done by leveraging resources and working with a broad team of experts from industry, national laboratories, government contractors, universities, stakeholders, and U.S. Department of Energy.

The goal of the workshop was to further collaboration between EMSP researchers and TFA end-users in the areas of tank waste characterization, retrieval and pretreatment, and tanks remediation. TFA needs were conveyed to the researchers and interactions were established to transfer the research results to the end-user. Linkage to new and past TFA needs and points of contact were given. EMSP awardees discussed their research plans and received feedback from TFA Technical Integration Managers and safety personnel. Minutes from the breakout sessions summarize TFA questions, recommendations to the researchers, linkages to related tasks, and points of contact.

- *Detection and Characterization of Chemicals Present in Tank Waste* by Dr. P. G. Datskos* (ORNL) and Dr. Sepaniak (Univ. of Tenn.)

  Questions:
  - How do you keep the sensor clean?
  - What is the effect of the tank contents (i.e., caustic, acidic, etc.) on the coating?
  - Is there an upper limit for temperatures?
  - How does radioactivity effect the electronics?

  TFA Recommendation:
  - There is a need for at-tank rather than in-tank characterization.
  - Look at organics at low-levels (ppm) rather than bulk constituents.
  - Look at suitable analytes.

- *Correlation of Chemisorption and Electronic Effects for Metal/Oxide Interfaces: Transducing Principles for Temperature Programmed Gas Microsensors* by Dr. Semancik & Dr. Tarlov (NIST), Dr. McAvoy & Dr. Suehle (U of Maryland) - presented by Richard Cavicchi (NIST)

  Questions:
  - Is it reversible?
  - Can it be made quantitative?
  - What are the levels of detection?

  TFA Recommendation:
  - No site needs submitted to TFA for tank head-space monitor development in 1995-1998 time period. 8/95 discussions with Hanford project manager for head space gas analysis in tank SY101 indicated that WHC was satisfied with

IR, GC, & H_2 chemical cell monitoring of the vent off-gas. CMST pursued the question of in-tank head-space H_2 monitoring with the TFA in 5/96 and found no apparent need at Hanford.

– There is a potential application for this technology in the Mixed Waste Focus Area for incinerator off-gas monitoring.

- *Mass Spectrometric Fingerprinting of Tank Waste Using Tunable Ultrafast Infrared Lasers* by Dr. Haglund (Vanderbilt University) and Dr. Wayne Hess (PNNL)

  Questions:
  – Can it be made quantitative?

  TFA Recommendation:
  – The usefulness of this tool is for quantitative (molecular species) measurements of organics in solids.

- *Electrically Driven Technologies for Radioactive Aerosol Abatement* by O.A. Ezekoye (University of Texas)

  – No linkage found within the TFA.
  – Potential end-users of this technology might be found in the following areas: calcine off-gas, vitrification, and spent nuclear fuel.
  – Other potential applications, such as medical applications, might be found by reviewing the proceedings of the Nuclear Air Cleaning Conference.

- *Precipitation and Disposition of Aluminum-Containing Phases in Tank Waste* presented by Jun Liu representing the collaboration of Baskron, Virden, Wang, and Keefer from PNNL with Hobbs from SRTC and with Dabbs and Aksay from Princeton.

  The TFA asked Jun if he could/would analyze a specimen of the 101 SY tank crust, if he had it. The TFA, Randy Kirkbride, Andy Felmy, and Jun engaged in a discussion about the ability to get this data into the form of information that could be used in the ESP model.

- *Solution Effects on Cesium Complexation with Calixerene Crown Ethers from Liquid to Supercritical Fluids* presented by Chien Wai of the University of Idaho.

  Most of the subsequent discussion centered on the viability of a process that operates at 75 atmospheres in a nuclear environment. This concern has hampered efforts to employ this type of technology in other waste management arenas such as mixed waste. The TFA contends that it is not likely to pass the safety analysis reviews in the foreseeable future. Chien Wai indicated that he would refocus the program to use his experiments to elucidate dissolution mechanisms.

- *Graduate Students* was presented by Yasuo Onishi (PNNL) representing a large number of collaborators: Felmy, Rustad, Recknagle, Michener, Fann (PNNL); Jordon (IBM); Liu (CRAY-SGI Research); and Yuen (University of Minnesota).

TFA asked if differing tank geometries could be included in the model and was reassured that this was the case. TFA indicated that they had funded some tank settling tests for C-106, C-107, and S-106 and would like this data to be used in the model. TFA indicated a desire to have Onishi collaborate with Florida International University in their upcoming line plugging tests.

Characterization, Monitoring and Sensor Technology Crosscutting Program (CMST-CP)
Annual Review
March 8-11, 1999
Gaithersburg, MD

Thirty-three people attended the EMSP Presentations during the CMST-CP Annual Review. Eighteen attendees were associated with the EMSP and 15 others were from CMST-CP, Focus Areas (FAs), the Nuclear Regulatory Commission, and FETC. There was much interest in the EMSP research by CMST and the FAs.

Eleven EMSP projects and one Wolf-Broido project were presented. There were four research projects on the subject of laser ablation — the researchers were knowledgeable about what the other researchers were doing in the area and formed their own collaborations. A fact sheet describing each project scheduled for presentations was prepared for each EMSP presenter and made available to the CMST-CP Review prior to the presentations. The FA/CP personnel read the information on the fact sheets prior to the EMSP presentations so that they would have some background on the projects and could decide which presentations they wanted to attend. Boris Fabyschenko from LBL distributed a press release on the application of chaos theory to fractured media. Andrew Pipino from NIST displayed a poster on the Evanescent Wave Cavity Ring-Down Miniature Spectrometer in the back of the meeting room. Mark Pickrell from LANL addressed transfer of his mature research project, which has developed a neutron source; two commercial partners have subsequently applied for a license. Four laser ablation research projects were presented (Rick Russo, Scott Goode, Mike Anderson, and Mike Pellin) and CMST expressed interest in perhaps integrating these projects into a follow-on technology development effort.

The banquet was well attended (28 people) and there was a lot of interchange during dinner. The reception afterwards at the hotel provided an opportunity to meet with the researchers and learn more about how to transition their research.

The Environmental Measurements Laboratory (EML) visit was informative and a good opportunity to get to know the DOE/NV CMST manager, the EML personnel, and EMSP researchers and learn about the research conducted by EML. EML will be performing quality assessments and project facilitation for CMST. Close contact between the CMST PIs and the project facilitators keeps the CMST projects on track and aligned with FA/Crosscut needs.

Subsurface Contaminants Focus Area (SCFA) Mid-Year Review
April 26-29, 1999
Augusta, GA

An EMSP room was set-up and over 20 PIs presented posters of their vadose zone work. The poster sessions were well attended. PIs had the opportunity to attend presentations by site personnel discussing current vadose zone cleanup activities.

A special session was held for PIs that was attended by the program manager of the EMSP, Mark Gilbertson, and Tom Hicks from SCFA. Discussions centered around general project descriptions, the SCFA path forward for incorporating EMSP projects in the Focus Area, and PI feedback to Mark Gilbertson. Several of the PIs voiced their support of the recent EMSP research integration efforts including the topical workshops and participation with the Focus Areas.

Deactivation and Decommissioning Focus Area (DDFA) Mid-Year Review
May 25-27, 1999
Morgantown, WV

At the request of the DDFA, the Environmental Management Science Program (EMSP) attended and participated in the DDFA Mid-Year Review. Chester Miller of the DOE-HQ made presentations for 21 of the 22 EMSP projects related to DDFA. Dr. Bernard Cooper of the University of West Virginia attended and presented his project. Posters for 8 EMSP DDFA related projects were displayed.

Dr. Cooper indicated that his project is now at a point that he needs someone as a "broker" to help progress it to the next step. He feels that the next step will be to perform field-testing. He is also interested in testing his methods on plutonium/ uranium samples.

Dr. William Stone of NIST expressed interest in Dr. George Xu's presentation on "Real-Time Identification and Characterization of Asbestos and Concrete Materials with Radioactive Contamination". He was provided with a copy of Dr. Xu's presentations, poster and contact information.

The EMSP Staff met with Robert Vagnetti from the DDFA to establish a dialogue on how the EMSP could best support the DDFA in the future and how to make our gap analyses more useful. Mr. Vagnetti indicated that he would be willing to review our current gap analysis and help in efforts for possible research integration.

American Chemical Society (ACS)
August 22-26, 1999
New Orleans, Louisiana

The EMSP will have a strong presence at the ACS Meeting with 120 presentations in 8 technical sessions dedicated to EMSP projects. There will also be 2 tutorials, a plenary session, and 2 poster sessions. A poster on research integration for the EMSP will be presented by EMSP staff. This will provide a forum for researcher interaction among EMSP researchers and non-EMSP funded researchers. A large fraction of the EMSP portfolio addresses research that deals with actinide chemistry issues faced by DOE.

* presenter

Oak Ridge Operations Environmental Management Science Program Workshop September 22, 1999 Oak Ridge, TN

The purposes of this workshop were to inform EMSP principal investigators of the Oak Operations Office's (ORO) environmental cleanup needs, introduce end-users to EMSP projects that have relevance to ORO needs, and to cultivate collaborations and other relationships between the participants. More than seventy attendees participated in the workshop, including: EMSP researchers; representatives from the Site Technology Coordination Group, Subsurface Contaminants Focus Area, state regulators, and public stakeholder groups; end-users from the major sites administered by the Oak Operations Office; and EMSP staff.

The day's activities began with a short bus tour of two of the three sites that encompass the Oak Ridge Reservation (ORR), the East Tennessee Technology Park and Y-12 Site. The group reconvened at the conference center for a warm Tennessee welcome by the Oak Ridge Operations Office, an introduction to the EMSP, and presentations by the various end-users about their site problems. The sites discussed included the Paducah Gaseous Diffusion Plant, the Portsmouth Gaseous Diffusion Plant, the Y-12 Site, the Oak Ridge National Laboratory (ORNL), and the East Tennessee Technology Park (ETTP, formerly the K-25 Site). After lunch, the participants were guided into one of four breakout sessions where researchers presented their work and discussions about how it related to site needs ensued. The breakout session topics were: 1) D&D Characterization, Decontamination, and Recycle; 2) Soil and Groundwater Treatment; 3) Subsurface Imaging and Characterization; and 4) Bioremediation. Researchers were selected to present their work based on their project's relevancy to ORO cleanup needs.

Interactions between PIs and end-users included the following:

- Dr. A. J. Francis (Brookhaven National Laboratory) and Dr. Gary Halada (SUNY at Stony Brook) began discussions with Gary Person about testing their D&D techniques on materials at ETTP. Their project is titled "Mechanisms of Radionuclide-Hydroxycarboxylic Acid Interactions for Decontamination of Metallic Surfaces."

- Dr. Sherman Ponder started discussions with Jerry Harness, representing the Efficient Separations Crosscutting Program, about possible use of Dr. Ponder's unique separations technology. Dr. Ponder's project is titled "Removal of Technetium, Carbon Tetrachloride, and Metals from DOE Properties."

- Dr. Ernest Majer's presentation, "Subsurface High Resolution Definition Of Subsurface Heterogeniety For Understanding The Biodynamics Of Natural Field Systems: Advancing The Ability For Scaling To Field

Conditions", sparked interest by the Subsurface Contaminants Focus Area DNAPLs Product Line Manager, Elizabeth Phillips. They will continue discussions in an effort to collaborate in the future on some bioremediation work.

The site tour generated further interest in seeing more detail about ORNL's subsurface contamination and decontamination and decommissioning projects. A follow-on tour is now being arranged for ORNL principal investigators to meet with team leads for these projects.

Nuclear Materials Focus Area EMSP Actinide Chemistry Workshop
November 9-10, 1999
Albuquerque, NM

This workshop brought EMSP principal investigators in contact with representatives and researchers from the Nuclear Materials Focus Area, Nuclear Materials Lead Laboratory, Seaborg Institute, and the Plutonium Center. Research presented during this two-day workshop was designed to highlight current activities related to actinide chemistry of plutonium stabilization, actinides in the subsurface, and actinides solution separations.

Twelve EMSP oral presentations were made, and approximately 20 posters were displayed representing other EMSP research. Topical sessions included in this workshop were:

- Program Overviews
- Clean-up/Decontamination Methods
- Behavior in Groundwater and Soils
- Actinide Behavior in High-level and Other Wastes
- Surveillance, Monitoring, Characterization, and Sensor Development
- Actinide Separations Chemistry and Techniques.

The workshop was attended by more than 40 registered individuals, and due to the close proximity with Sandia National Laboratory, Los Alamos National Laboratory, and The University of New Mexico, numerous non-registered attendees came to selected sessions. As an added activity, attendees were given the opportunity to comment on the EMSP program. At least 10 specific action items were recommended for program improvement.

The workshop ended on a positive note with all participants agreeing that meetings of this type were beneficial and provided opportunities for information exchange related to program needs and areas of promising research and technology development.

Kickoff Workshop for the 1999 Environmental Management Science Program Vadose Zone Research Awards
November 16-18, 1999
Richland, WA

These proceedings document the Kickoff Workshop for the 1999 Environmental Management Science Program Vadose Zone Research Awards. The workshop attendees were comprised of researchers, Focus Area representatives, EMSP staff, and science and technology endusers. Three integration teams were formed: (1) Waste/Sediment Lab Experiments and Process Models, (2) Vadose Zone Transport Field Studies, Advanced Characterization, and Transport Modeling, and (3) Monitoring and Remediation at Hanford and Across the Complex. The researchers had the opportunity to listen to talks given by Focus Area representatives, EMSP staff, and science and technology endusers and to present their proposed research plans. The purpose of holding the workshop at the outset of the award process is to give the PIs critical information necessary to direct their research towards the most useful avenues, make available existing data and models, involve the PIs in plans for future vadose zone activities, encourage collaboration among researchers and with endusers, and provide feedback to maximize the benefit of the research. The nucleus of each of these three integration teams will be kept intact through a series of follow-on workshops. The first of these follow-on workshops, which will address collaboration relative to vadose zone characterization, is scheduled for January 20-21, 2000 in Richland, WA.

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News Releases

NEWS RELEASES

Several EMSP-sponsored technology development projects have been highlighted in news releases since the inception of the EM Science Program. Examples of these are included below.

EMSP: Basic Research to Solve Cleanup Needs

What has the Environmental Management Science Program (EMSP) accomplished in three years? Since its beginning in fiscal year 1996, this collaboration between the U.S. Department of Energy's offices of Energy Research and Environmental Management has invested over $160 million to support 202 research projects. Fiscal year 1998 grants will be awarded this summer to respond to two need areas: decontamination and decommissioning and high-level radioactive waste. Scientists funded through EMSP are currently conducting research at 70 universities, 13 DOE laboratories, and 12 other governmental and private laboratories located in 34 states, Canada, and Australia. EMSP research grants last three years.

But EMSP has accomplished more than providing research dollars. The longer-term basic science program was established in response to a congressional mandate to expand scientific and engineering knowledge in order to replace current conventional approaches, which are often costly and ineffective, with new and innovative cleanup methods. In addition to its funding role, EMSP has established a framework to enable DOE to capitalize on its scientific research investments.

Among the elements of this framework are the following:

- Ensuring that funded proposals have both scientific merit and relevance to cleanup needs at sites and across the complex. EMSP's research portfolio addresses the most challenging technical problems of the Environmental Management Program related to high-level waste; spent nuclear fuel; mixed waste; nuclear materials; remedial action; decontamination and decommissioning; and health, ecology, or risk (a crosscutting area).

- Ensuring that the six technical problem areas and the crosscutting area are funded at appropriate levels. With each new solicitation, EMSP has an opportunity to tailor requests for proposals to equitably support its hierarchy of needs. The program has organized its 202 funded research projects within a framework that shows how the projects relate to 13 scientific disciplines, the six EM problem areas, and the 353 high-cost and high-risk projects described in the draft Accelerating Cleanup: Paths to Closure document. This exercise has helped the program determine how high-priority needs are being served through funded research and helps guide future funding decisions.

- Using advisory groups such as the Environmental Management Advisory Board's Science Committee, the Strategic Laboratory Council, and the National Academy of Sciences/ National Research Council to improve the quality of the program and the process for selecting proposals.

- Establishing a plan for dissemination of research results to site problem holders. The first phase of the dissemination plan is a workshop in Chicago in July 1998 that will bring together researchers and site problem holders to share research results, research needs, and site problems.

The DOE Idaho Operations Office at the Idaho National Engineering and Environmental Laboratory coordinates contractual details of the grants and is responsible for integrating results among researchers and DOE representatives. Results of research conducted under the first year of funding will soon become available, and mechanisms are being developed to share that information with DOE site representatives and other interested stakeholders.

For more information on EMSP and its funded projects, see the program's Web sites at http://emsp.em.doe.gov.

Building a Wall of Bacteria

Through the Environmental Management Science Program (EMSP), DOE's Office of Environmental Management (EM) and Office of Science (SC) collaborate to fund basic research to solve intractable problems that threaten the successful closure of DOE sites. As one of the programs within the Office of Science and Technology, EMSP ensures that OST's projects cover the full spectrum of R&D.

Containment barriers can significantly shorten the schedule and reduce the cost of subsurface remediation by slowing or stopping the movement of contaminants through soil. To optimize the ability of active biowalls to contain priority contaminants on DOE sites, scientists need a greater understanding of microbial, geochemical, and hydrogeological processes that interact and often compete.

An EMSP project titled "Containment of Toxic Metals and Radionuclides in Porous and Fractured Media: Optimizing Biogeochemical Reduction versus Geochemical Oxidation" is providing basic knowledge about the optimal conditions for bacteria to immobilize certain contaminants. The study, led by Oak Ridge National Laboratory's Phil Jardine and Scott Brooks, is motivated by the likelihood that subsurface microbial activity can alter the state of toxic metals and radionuclides so that they are immobilized and contained for the long term.

Graphics provided by Oak Ridge National Laboratory

Working in an anaerobic chamber, Scott Brooks prepares a column displacement experiment to investigate the immobilization of toxic metals and radionuclides by metal-reducing bacteria.

The project's overall goal is to understand and model the mechanisms whereby metal-reducing bacteria aid the stabilization of these contaminants in porous soil. Results could lead directly to cost-effective strategies for active biowalls in ongoing or planned remediation projects at Hanford's In Situ Redox Manipulation site, Savannah River's Old Burial Ground, and sites at Oak Ridge's Y-12 Plant.

The study's three multidisciplinary tasks build on collaborations established years ago within DOE's Subsurface Science Program:

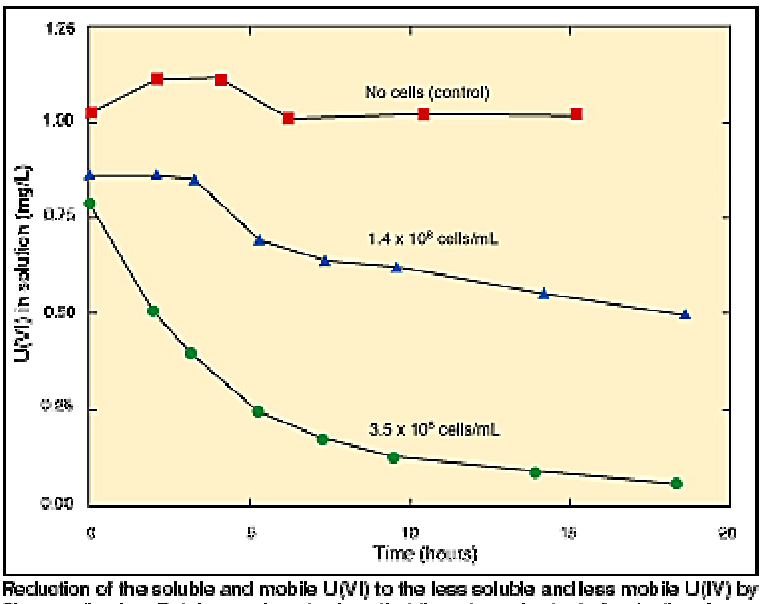
- Jardine, Brooks, and their ORNL associates are using a dynamic flow technique to quantify rates of oxidation and reduction and mechanisms controlling the mobility of uranium, chromium, and cobalt-EDTA (ethylenediaminetetraacetic acid).

- Stanford University's Scott Fendorf uses X-ray absorption spectroscopy (XAS) at the Stanford Synchrotron Radiation Laboratory to measure the redox transformation and immobilization of these contaminants by subsurface media.

- Finally, James Saiers, formerly of Florida International University and now at Yale, is using the experimental data to develop computer models that simulate hydrologic-biogeochemical transport processes.

The Electron Tug-of-War

When the contaminants of concern contact metal oxides indigenous to the soil, the contaminants undergo geochemical oxidation (lose electrons). The resulting ions with higher valences—U(VI), Cr(VI), and 60Co(III)EDTA—are dangerous for a variety of reasons. The chromium is more toxic, and all three are more readily dissolved in and spread by migrating groundwater. But scientists have discovered a number of bacteria whose metabolic processes affect the redox state of toxic metals and radionuclides. When the contaminants are reduced (gain electrons, so that their positive charges decrease), the resulting ions—U(IV), Cr(III), and 60Co(II)EDTA—are less soluble. Instead of being transported by groundwater, they sorb to neighboring soils and sediments. This project has tackled the challenges of sustaining microbial reduction processes in situ for long periods of time and optimizing the processes in spite of competing geochemical oxidation and sorption reactions.



Reduction of the soluble and mobile U(VI) to the less soluble and less mobile U(IV) by Shewanella alga. Batch experiments show that the rate and extent of reduction depends on the number of bacterial cells in the suspension. The lack of reduction in the control (no cell) experiments confirms that the bacteria are required for the reduction reaction to occur.

The dynamic flow experiments are performed by sending solutions up through columns of simulated soils containing pure mineral oxides and of heterogeneous soils and sediments from Oak Ridge, Savannah River, and Hanford sites. Jardine reports that Brooks was the first to demonstrate the sustained microbial reduction of 60Co(III)EDTA to 60Co(II)EDTA under dynamic flow conditions. “After discovering a way to keep the bacteria healthy and growing, we were able to effectively stabilize 60Co(II)EDTA in a flowing system, even in the presence of strong mineral oxidants like manganese and iron oxides commonly found in the subsurface.”

Experiments with uranium are focused on the effects of geochemical oxidation and interfacial sorption reactions and the effects of biological reduction processes on mobility rates of uranium in the actual site sediments. Because XAS is sensitive to metal redox shifts and interfacial surface reactions, the researchers use it to quantify the time-dependent bacterial reduction of U(VI) to U(IV) for a variety of environmental conditions. The transformation has proven generally quite rapid, with time scales of hours or even minutes.

Problem Solving, Number Crunching, and Beyond

Toxicity presents problems for bacterial reduction of chromium to the less toxic and mobile species, but project personnel have discovered two alternative methods. The first is a direct, abiotic process in which natural organic matter (NOM) reduces Cr(VI) to Cr(III), slowing its subsurface mobility by many orders of magnitude. NOM’s ready sorbancy to soils and sediments makes this a promising technique for efficient, cost-effective geochemical barriers. The second method is indirect: bacteria reduce iron oxides to Fe(II), which in turn quickly reduces Cr(VI) to Cr(III). This catalytic process, in which the only reactant lost is Cr(VI), shows promise for use in active biowalls for the in situ containment of chromium. Both techniques have been quantified using time-resolved XAS.

Jardine reports that efforts in this third and final year of the project focus on troubleshooting the uranium system and computer modeling. The bacteria (Shewanella alga) are forming U(IV), but sustained growth during dynamic flow has been problematic.

Experimental data already derived are being crunched by the team's computer specialist into a biohydrogeochemical model whose calibrated code can assist with various DOE site needs. The team hopes the next step will be a field-scale bioreduction demonstration at a field facility developed at ORNL to investigate groundwater flow and transport processes in fractured shale bedrock. For information on that facility, see www.esd.ornl.gov/facilities/hydrology/WAG5.

For further information, contact Phil Jardine, ORNL, (423) 576-8085, ipj@ornl.gov.

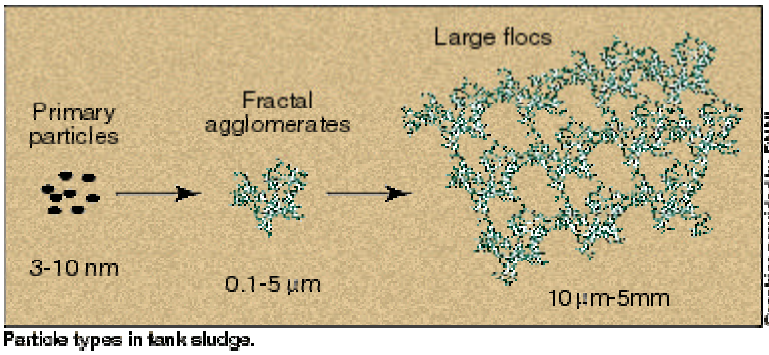
The Science of Sludge

The science of Sludge

Through the Environmental Management Science Program (EMSP), DOE's Office of Environmental Management (EM) and Office of Science (SC) collaborate to fund basic research to solve intractable problems that threaten the successful closure of DOE sites. As one of the offices within the Office of Science and Technology, EMSP ensures that OST's projects cover the full spectrum of R&D.

The millions of gallons of radioactive waste stored in underground tanks are a top-priority remediation problem for the U.S. Department of Energy. From a waste processing standpoint, the tank waste components of greatest concern are insoluble sludges consisting of suspensions of colloids, particles between a nanometer and micrometer in diameter.

Under common circumstances, the colloidal particles can form agglomerate networks that impede several aspects of waste processing. They can trap flammable gases, making retrieval and transport more dangerous. They can clog transfer lines and extraction systems like filters and ion exchangers. And they resist efficient sedimentation, frustrating efforts to reduce the volume of waste to be treated and disposed of.



Particle types in tank sludge.

Given the range of chemistries present in DOE tanks, it's impractical to measure the properties of all tank wastes under all potential conditions to design rational treatment procedures. Instead, a sound scientific framework for predicting property trends needs to be established. That's the goal of an Environmental Management Science Program project titled "Colloidal Agglomeration in Tank Sludge: Impact on Waste Processing." A team combining researchers from Pacific Northwest, Oak Ridge, and Sandia National Laboratories and the University of Washington is in the last year of this three-year project. The resulting enhanced understanding of agglomeration phenomena and the properties of complex colloidal suspensions will aid in the development of new methods and techniques for processing hazardous tank wastes.

Researchers are working to:

- understand the factors controlling the nature and extent of colloidal agglomeration under expected waste processing conditions;
- determine how agglomeration phenomena influence physical properties relevant to waste processing including rheology, sedimentation, and filtration; and
- develop strategies for optimizing processing conditions by controlling agglomeration phenomena.

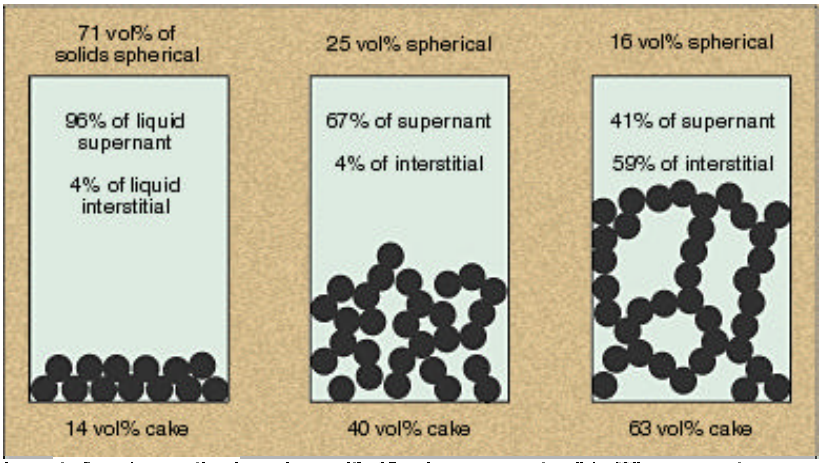
Significant Findings

Transmission electron microscopy of actual wastes shows that most sludges consist of agglomerates of submicrometer-sized primary particles of hydrated oxides and insoluble salts. To aid experimentation, researchers identified model colloid suspensions that duplicate the compositions and particle morphologies of actual waste. Static light scattering measurements on both model suspensions and actual wastes showed that the primary particles in the basic salt solutions found in most tank wastes undergo extensive aggregation to form fractal agglomerates. This structure has an enormous impact on slurry properties because fractal objects occupy much more space than dense objects at the same solids loading.

Depending on the extent of agglomeration and solids loading, slurry viscosities can vary by over five orders of magnitude, and the most viscous suspensions contain colloidal agglomerates. To achieve desired viscosities for retrieval and transport, these sludges require 20-fold dilution, producing enormous quantities of wastes.

The researchers have also found that primary particle and agglomerate size can influence sedimentation rates by over three orders of magnitude. Laboratory tests on actual tank wastes revealed that final sediment densities ranging from only 1 to 8 volume percent are common. This means that particulate layers will occupy large volumes during steps such as sludge washing and leaching and that the volume occupied by sediment layers is predominantly interstitial water that cannot be removed during solid-liquid separations.

Experiments have further indicated that the solids loading in sediment layers is highly dependent on the degree of agglomeration and the interparticle interaction potential. Packing of individual particles can be highly efficient (up to 50 volume percent). For agglomerated systems, sediment densities are much lower, but can be increased up to threefold by weakening interparticle interactions. This increases the compressibility of the sediment, which compacts under its own weight. Experiments have shown that in the high-salt regime of most tank wastes, sediment densities first decrease, then increase with salt content because of the interplay of electrical double layer and hydration forces. The presence of calcium and other divalent cations is particularly effective in promoting sediment compression. Manipulation of such forces could be used to improve tank utilization and the efficiency of solid-liquid separations during steps such as sludge washing and leaching.



Impact of agglomeration in a slurry with 10 volume percent solids. When a greater portion of the solids is agglomerated rather than spherical, more interstitial liquid is trapped in the cake. The cake consequently occupies a larger portion of the tank, and less supernatant can be decanted for treatment.

"We can now predict sludge properties if we know the distributions of primary particle and agglomerate sizes present in a given tank," says initial principal investigator Bruce Bunker. "If tank sludges are properly characterized, we can predict processing conditions that are likely to be encountered. For example, we can predict solids loadings above which the contents of a given tank are likely to be transformed from pumpable liquids into viscous gels that will clog transfer lines." Unfortunately, it may not be practical to measure agglomerate distributions in certain radioactive

wastes. “Our long-term goal is to be able to predict agglomerate distributions based on interparticle interaction potentials, which are controlled by particle types and solution chemistry,” says Bunker.

Closing in on Practical Applications

While work to date suggests that short-range forces are important in controlling the properties of tank sludge, quantitative models do not yet exist to predict sludge properties such as sediment densities or slurry viscosities based solely on interaction potentials. Work in fiscal year 1999 is focused on measuring short-range forces, determining how different salts influence the fractal dimension and size of colloidal agglomerates, and modeling agglomerate properties. Once the framework relating interparticle forces, agglomeration, and sludge properties is established, the project will devise modifications of sludge suspensions to optimize properties for retrieval, transport, and sedimentation processes.

For further information, contact Joel Tingey, current principal investigator, PNNL, (509) 376-2580.

Science Program Project Builds a More Intense Neutron Source

Science Program project builds a more intense neutron source

The Environmental Management Science Program, a partnership between the Office of Environmental Management and the Office of Energy Research, was chartered by Congress in 1996 to fund targeted research for the development of breakthrough approaches for solving DOE's environmental problems with less expense, on accelerated schedules, and at less risk to workers and the public. EMSP projects provide EM with basic research for fundamental data that may be critical to advancing technologies under development but not yet implemented, and they generally address problems considered intractable without new knowledge.

EMSP projects are typified by the High-Fluence Neutron Source for Nondestructive Characterization of Nuclear Waste under development at Los Alamos National Laboratory. The goal of this project is to build an economical, compact, and transportable yet intense neutron source for applications in assaying nuclear and chemical waste, detecting high explosives, and supporting safeguards and nonproliferation applications.

Potential EM applications include characterizing transuranic wastes, particularly remote-handled wastes, for the Waste Isolation Pilot Plant and measuring high-level wastes, cemented or vitrified wastes, and residues prior to stabilization and disposal. Existing technology is insufficient to measure these contaminants because it addressed a substantially different technical problem: the measurement of very pure material. However, the present need is to develop measurement capability for highly impure, contaminated, and heterogeneous wastes and residues of the production process. One problem in particular is the measurement of wastes with very high radiation (neutron) backgrounds. These measurement conditions demand measurement capabilities several orders of magnitude above existing capabilities.

An intense neutron source directly addresses the need to characterize nuclear materials under difficult measurement conditions. The benefit of this approach is that mature, neutron-based, nondestructive characterization methods can be used, but their capabilities will be increased by the same amount as the increase in neutron intensity. The proposed neutron source could extend existing instrumentation sufficiently to meet these requirements.

The LANL team is researching the basic plasma physics necessary to develop a high-fluence neutron source based on the inertial electrostatically confined (IEC) plasma. This technology has potential for immediate application as a portable neutron source. IEC devices have significant advantages over present neutron sources in both cost and safety. The project goal is to develop a source that produces 1011 neutrons/second with a cost, weight, and size comparable to current systems, which are three orders of magnitude less powerful.

Photos provided by Los Alamos National Laboratory.

The two halves of the IEC vacuum chamber.

The IEC device, originally developed in the 1950s as a possible fusion reactor, operates as a deuterium-tritium neutron generator. The basic system is a spherical vacuum chamber containing a spherical grid. The grid is raised to a high negative potential. A breakdown develops

between the chamber wall and the grid, and this plasma becomes a source of positive deuterium and tritium ions. These ions are accelerated to the center of the vacuum chamber sphere where they may collide.

Early experimentation showed that neutron yield scaled inversely with density. In collisional operations, accelerated ions are likely to collide with fill gas neutrals in the accelerating grid interior. Therefore, the ions never achieve the full accelerating potential of the grid. A novel approach proposed at LANL removes this limitation by using a triple grid design, in which the inner grid is the accelerating grid. It is raised to high negative potential and serves the same function as the single grid in conventional IEC systems. The central grid serves as electrical isolation and is held at ground potential. The outer grid is raised to a modest positive potential.

Electrons are injected by six dispenser cathodes around the 12-inch-diameter vacuum chamber. The electrons are trapped and orbit around the outer grid, ionizing a local plasma. Because of the modest potential, the breakdown occurs at a much lower density. The limit is further relaxed by the injected ionization from the dispenser cathodes. The result is a lower density plasma, which diffuses across the second grid and is rapidly accelerated by the inner grid. As the density is reduced, the plasma becomes collisionless. The result is a tight focus of fully accelerated ions, with large collision energy and neutron yield.


Adjusting components on the IEC vacuum chamber.

The LANL project team has completed construction of the IEC device, and all systems are fully functional. Experimental operations are under way to "tune" the system to deal with plasma arcing problems and to raise the main accelerating voltage to its full 75-kilovolt potential. The design goal of this phase is production of 109 n/s, operating in pure deuterium, which can be vented in a normal vacuum system. Principal investigator Mark Pickrell expects the system to achieve this goal in the early months of 1999.

Once operating parameters are established, the working design will be frozen, and tritium operations will begin. Since tritium is radioactive, the system will be completely sealed, and the vacuum system will no longer vent. This operating regime should generate the ultimate goal of 1011 n/s. The LANL project team would eventually like to see an industrial private-sector partner convert the IEC system from a laboratory experiment to an commercially available industrial machine.

For more information about the High-Fluence Neutron Source for Nondestructive Characterization of Nuclear Waste project, contact Mark Pickrell at LANL, (505) 665-5098, mpickrell@lanl.gov.
Simpler. Cheaper. Better!

Through the Environmental Management Science Program (EMSP), DOE's Office of Environmental Management (EM) and Office of Science (SC) collaborate to fund basic research to solve intractable problems that threaten the successful closure of DOE sites. As one of the programs within the Office of Science and Technology, EMSP ensures that OST's projects cover the full spectrum of R&D.

One of DOE's primary remediation challenges is the safe and cost-effective disposal of radioactive wastes currently stored in underground tanks at the Hanford, Oak Ridge, and Savannah River sites. Waste forms must be chemically durable under environmental storage conditions and thermally stable under repository conditions over a geologic time scale. The remediation plan for Hanford's 177 tanks calls for disposal of highly radioactive waste in the form of borosilicate glass "logs."

Simpler. Cheaper. Better!

Simpler. Cheaper. Better!

EMSP project explores alternative waste form for ion exchangers

To make processing practical and to reduce the ultimate waste volume, radionuclides in the liquid above the tank sludges—principally cesium and strontium—must be precipitated or separated out. One of the most cesium-selective, stable ion exchangers is crystalline silicotitanate (CST), but borosilicate glass may not be the best waste form for disposing of the loaded ion exchangers, which are nonregenerable.

Titanium dioxide in the CST complicates the vitrification process and affects the quality of the waste form, but limiting its concentration to acceptable levels creates other problems. Because processing takes longer, interim storage is required, raising not only costs but safety issues as well. Dangerous levels of hydrogen may be generated in the wet, used ion exchangers while they await further processing. And the higher volume of the dilute final waste form drives up the expense of processing, transportation, and ultimate storage.

Beyond the issues of time and concentration, dissolving CST in borosilicate glass requires removal and transfer of CST from ion exchange columns, mixing it with glass frit, and melting—all steps that carry risk of contamination to workers and the environment. Moreover, cesium's volatility is a concern at the temperatures required for vitrification. All of these factors add up to the need for a better method to dispose of CST, one that requires less interim storage, handling, dilution, and heat. This need is all the more pressing because problems with precipitation processes are making separation increasingly the method of choice for treating liquid tank waste.

Finding a simpler solution

Researchers at Pacific Northwest National Laboratory are teamed with others from Sandia National Laboratories and the University of California at Davis in an EMSP project to explore new disposal strategies and waste forms specific to CST—in particular, in situ heat treatment. Direct thermal conversion of cesium-loaded CST ion exchangers is possible because they already contain basic ingredients that can form a ceramic or glass at high temperature. The project, entitled "New Silicotitanate Waste Forms: Development and Characterization," is generating information on the durability and stability of thermally consolidated CSTs to evaluate the viability of this option for storage and disposal.

Graphics provided by Pacific Northwest National Laboratory.

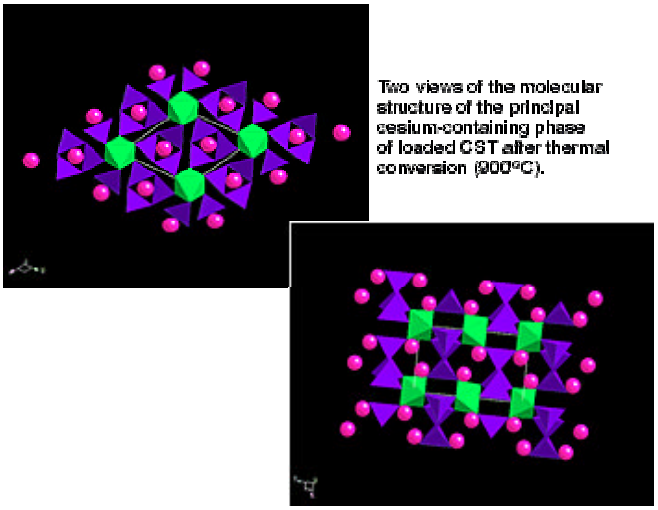
PNNL's Lou Balmer prepares solutions for ion exchange.

This approach would immobilize the radionuclides in the consolidated ion exchanger in a much simpler process with minimal handling and also remove the water and hydroxyl groups that permit radiolytic hydrogen generation during storage. The potential benefits are numerous and substantial:

- Eliminating handling steps would cut the risk of accidental contamination.
- Reducing or eliminating storage prior to treatment would save money and minimize the opportunity for hydrogen generation while waiting for final disposition.
- Waste requiring vitrification into borosilicate glass could be more concentrated and thus less voluminous, saving many millions of dollars in processing and storage costs.
- Lower processing temperatures would reduce issues related to cesium's volatility.

The project's research strategy is based on an understanding of ceramic and glass structures and phase stabilities. Experiments at PNNL during the first year of the three-year project showed that thermally converted CSTs have aqueous durability several orders of magnitude higher than borosilicate glass: seven-day leached concentrations of less than 0.01 g/L compared to more than 13 g/L. Heat treatments of 500 and 900°C yielded the most durable ceramics, but the last residual water and hydroxyl groups are not removed until 800°C. Therefore, treatment at 900°C produced the optimal combination of leach resistance and prevention of hydrogen formation from radiolytic decay. Less than 1 percent of the cesium is lost through volatility during such processing. While this rate will still require capture and further treatment, it is a small fraction of that experienced with vitrification.

Phase stability and crystal chemistry studies are vital to predicting short- and long-term performance of waste forms. In its second year, the project team focused on defining the cesium-containing phases and thermodynamic stabilities of compounds related to the ion-exchanged CST and the thermally converted oxides. Transmission electron microscopy revealed that the majority of the cesium is contained in a cesium/X/silicon oxide, where X is a proprietary component of the ion exchanger. With the aid of X-ray diffraction, the new compBound was found to have a hexagonal crystalline structure consisting of silica tetrahedra and X octahedra, forming three- and six-membered rings (see graphic below). That the largest free aperture of the rings is smaller than a cesium atom accounts in part for the waste form's demonstrated high resistance to cesium leaching.



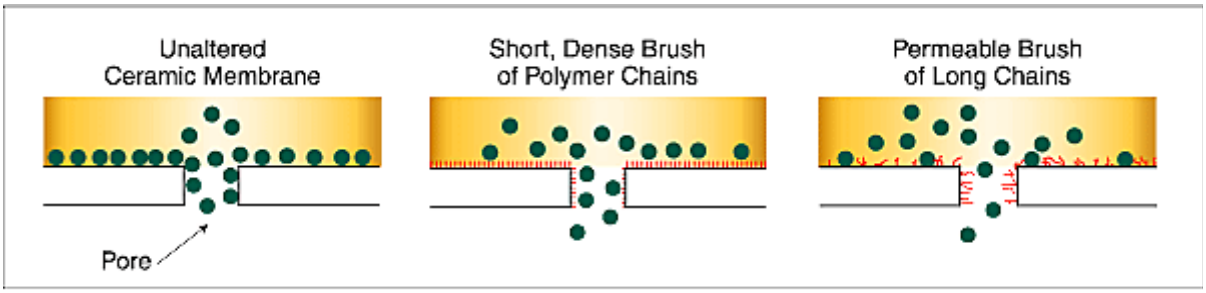
Two views of the molecular structure of the principal cesium-containing phase of loaded CST after thermal conversion (900°C).

Principal investigator Lou Balmerof PNNL reports that phase identification is nearly complete. SNL researchers are currently studying metastable phases to complete the team's understanding of the phase development during conversion to a stable ceramic waste form. Researchers at UC Davis are using solution-drop calorimetry to evaluate the thermodynamic stability of compounds fabricated at PNNL and SNL. The researchers aim to have, by the project's end, sufficient predictive capability to provide the basis for developing and controlling a process to dispose of CST ion exchangers that is not only technically sound, but faster, safer, and substantially more cost-effective than existing alternatives.

If the process is found feasible and applied at sites throughout the complex treating radioactive tank waste, reductions in risk, schedule, and cost could be very important. For further information on this research, contact Lou Balmer, PNNL, (509) 376-2006, lou.balmer@pnl.gov.

Creating a better membrane with ceramic-polymer composites

An Environmental Management Science Program project is developing and testing new tougher membranes that selectively separate and concentrate a target species, often present in dilute solution. These robust membranes made of ceramic-supported polymers (CSP) have the potential to perform difficult liquid-phase separations while consuming less energy than conventional distillation and extraction.



Graft polymerization modifies the pore surface of ceramic membranes.

Scientists at the University of California at Los Angeles have been working to advance the ability to "tailor design" a new class of tougher, task-specific CSP membranes for remediation applications, recovery and recycle, effluent treatment, and replacement of some energy-intensive separation processes. Led by UCLA's Yoram Cohen, researchers are developing chemically modified ceramic membranes for the treatment of oil-in-water emulsions and for the pervaporation removal of volatile organics from aqueous systems.

It gets hairy!

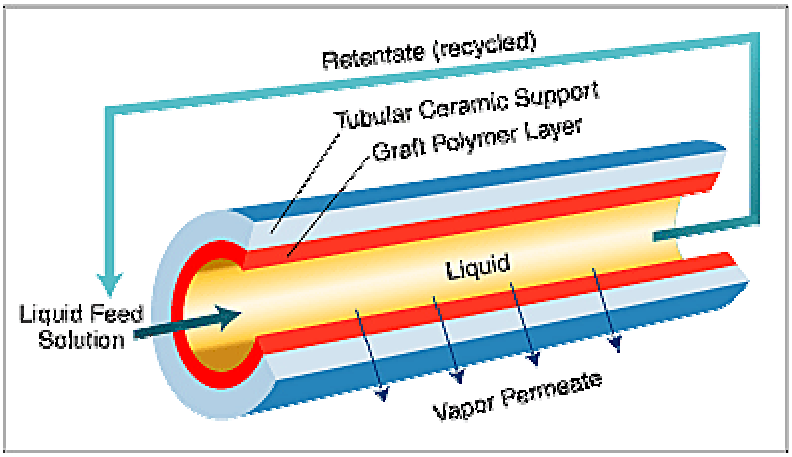
CSP membranes are fabricated by modifying the pore surface of a ceramic membrane support by a graft polymerization process. The process consists of activating the membrane surface with alkoxy vinyl silanes onto which vinyl monomers are added through free-radical graft polymerization, resulting in a thin surface layer of terminally anchored polymer chains. Reaction conditions are selected based on knowledge of the graft polymerization kinetics for the specific polymer/substrate system. The resulting CSP membrane is a composite structure whose mechanical strength and thermal stability are provided by the ceramic support and whose selectivity is determined by the covalently bonded polymer brush layer. What's unique about the CSP membrane, says Cohen, is that "the polymer membrane phase can be completely swollen by the solvent or permeate without a loss of membrane functionality. This is a clear advantage over current polymer membranes, whose performance degrades in harsh solvent conditions and high temperatures."

Synthesizing the membrane requires controlling the polymer surface graft yield and the length of the resulting terminally anchored surface chains by careful surface activation and control of the graft polymerization reaction. One prototype membrane featured highly hydrophilic polyvinylpyrrolidone (PVP) on a silica substrate. Because of its affinity for water (it is completely water soluble), the PVP brush layer expanded while preferentially allowing the passage of water over oil and improving separation performance.

Pervaporation removes organic contaminants

Another promising application of CSP membranes involves pervaporation, in which organic pollutants are removed from dilute aqueous waste by selective partitioning (solvation) into and diffusion through a polymeric membrane, followed by recovery as condensed vapor on the permeate side. Composite polymer

membranes have high selectivities but lack physical stability and are chemically vulnerable to various industrial solvents. Conversely, ceramic membranes have excellent structural integrity and high chemical and thermal resistance but poor selectivity and a limited selection of pore sizes. By modifying the surface of a ceramic substrate with a polymeric active layer, CSP membranes use the strengths of each approach to overcome the weaknesses of the other.



In pervaporation, polutants diffuse through the membrane as vapor.

A series of studies showed that polyvinyl acetate CSP membranes can separate and recover trichloroethylene (TCE), chloroform, and methyl tertiary butyl ether from aqueous solutions. Membrane pervaporation performance proved to be independent of solute concentration and period of usage and limited only by the feed-side concentration boundary layer. Experiments also found that the enrichment factor increased with increasing polymer graft yield. The enrichment factor for separation of TCE and chloroform from water varied from 69 to 150. The CSP membranes are ready for testing and scale-up for field applications. CSP membranes could be adapted for large-scale applications using available arrays of tubular membranes or a multichannel membrane assembly. Continuing research is focused on exploring a higher range of polymer surface densities and different choices of grafted polymer, more fully understanding the mechanism of CSP pervaporation, and optimizing the membranes for increased selectivity. Cohen says the ultimate goal is to "develop a membrane technology that can be used for organic-organic separations to replace energy-intensive separation processes like distillation and those using solvents for extraction. Clearly such replacements will be selective, but the benefit of pollution prevention would be immense."

For contact and other additional information, see the Web site of UCLA's Polymer and Separations Research Laboratory at http://www.polysep.ucla.edu.

New EMSP projects address subsurface cleanup problems

In September DOE Under Secretary of Energy Ernest Moniz announced funding totaling over $25 million for 31 new research projects tackling complex subsurface contamination problems. This is the fourth year of grants and other awards made under the department's Environmental Management Science Program, established by Congress in fiscal year 1996.

Many of the projects are collaborations among researchers at 20 universities, eight DOE labs, and three other research institutions. Nine projects will develop characterization and monitoring technologies to better understand the location and specific chemical nature of the contaminants; eight projects will help develop cost-effective, environmentally benign methods to remove radioactive contaminants from polluted sites; and 14 projects will study contaminant fate and transport to better understand how contaminants interact with and migrate through the soil and groundwater.

A complete list of the projects, including funding and research summaries, is available on EMSP's Web site at http://emsp.em.doe.gov.

Using Bacteria to Clean Up Subsurface Toxic and Radioactive Contamination

Scientists at the Department of Energy's Oak Ridge National Laboratory have shown that bacteria may be useful in preventing the spread of underground water contaminated by radioactive uranium, cobalt, and toxic chromium. Their research may reveal ways to protect the environment near contaminated waste disposal sites.

Philip Jardine and Scott Brooks are co-investigators studying how to chemically change chromium, cobalt and uranium into more manageable forms for cleanup. Brooks and Jardine imagine a "biowall," of bacteria actively reducing these highly mobile contaminants to a state in which they can be contained. "We envision that this would be a low-cost way to contain plume contamination. The big bucks would then be used to clean up the trenches," said Brooks. The two scientists and their colleagues are trying to stop these toxic chemicals from being transported any further in an environment that is actively transporting them.

Contamination originated through the now-abandoned practice of burying toxic metals and radioactive wastes in shallow, lined or unlined pits and trenches. Over the years, metals and radioactive wastes escaped into adjacent soils and groundwater. To protect the environment, scientists need to know how the contaminants move, and what can cause them to stop moving so that they can be cleaned up.

What researchers do know is that the subsurface environment is complex and variable. Rain percolates downward through soil and rock. Water can flow laterally through the soil and rock, carrying dissolved minerals and chemical compounds with it. Organisms in both the soil and water can use the dissolved material, and some compounds become fixed to organic matter. Oxygen in the water can change the chemical state of elements moving with the groundwater. It is through this complex environment that the contaminants escaped and continue to move.

The research focused on chromium, cobalt and uranium because these three elements can exist in several forms that affect their toxicity and the ease with which they can be cleaned up. "Chromium six" is both toxic and highly soluble, and can move freely in the subsurface environment. "Chromium three" is less toxic, has lower solubility and is therefore less mobile. Ideally, researchers would like to find a way to change (reduce) all the chromium six to chromium three.

Radioactive cobalt forms complexes with a substance called EDTA, a chemical agent used to remove scale that builds up in nuclear reactors and "hot" or radioactive cells. In one form, Cobalt and EDTA are soluble and can move with flowing water, in another form the chemicals tend to stick to soil particles and stay in place. The sticky cobalt and EDTA compound make the cleanup easier.

Uranium travels in groundwater as "uranium four" and "uranium six." Under most conditions the latter is extremely mobile in near-surface water containing oxygen, but under other conditions, it sticks to soil particles. Uranium four is less soluble and is easier to clean up.

They enlisted the aid of a bacterium, *Shewanella alga*, which can change (reduce) uranium six to uranium four, and the cobalt and EDTA compound into the sticky form. At Oak Ridge, Brooks tested the bacteria in an experiment column that simulated the soil and moving water of the subsurface. He put uranium six and a cobalt and EDTA compound in one end, and out came uranium four and the sticky cobalt and EDTA at the other. "One of the best things with Scott's work—and we didn't know it would work—was that he showed that we can maintain reduction of contaminants in the real world of flow," said his colleague Jardine.

Chromium proved to be difficult to study because the highly-toxic form—chromium six—killed the bacteria Brooks and Jardine were hoping would reduce it to chromium three. But they learned that iron oxides in soils can do the work of bacteria and change chromium six to chromium three.

They confirmed that *Shewanella* reduced cobalt and uranium by examining the soils and contaminants in tightly parallel beams of X-rays in the Stanford Synchrotron Radiation Laboratory. This process—X-ray Absorption Spectroscopy (XAS)—can distinguish the particular form of an element, and can identify the nearest atoms on the surface of soil grains, for example. It gives a 3-D picture of what is going on chemically, and of how the element of interest sticks to the soil. "We have put the flow mechanism in the beam and can write equations for what is going on," said Jardine. "One of the beauties of the technology," added Brooks, "is that it requires only a few atoms on the surface, for the technology can identify a thin layer of atoms."

"The whole design of the project was to have three intersecting studies," said Jardine, "molecular scale surface reactions (XAS), writing equations for modeling to obtain understanding, so that we can take it to the next level—field studies." He and Brooks now plan to use an Oak Ridge field facility for studying groundwater flow and transport processes in fractured rock beneath the surface. "We have shown sustainable microbial reduction of contaminants in a flowing system," said Jardine. "But the idea is for field application, to see if we can stimulate biological activity in the subsurface to sustain the reaction. We feel we're ready to go out and demonstrate it."

This work is supported by the U.S. Department of Energy Environmental Management Science Program (EMSP). The EMSP funds basic research through a partnership between the Office of Environmental Management (EM) and the Office of Science (SC) in the Department of Energy. The intent of the EMSP is to develop the scientific knowledge needed to create new technologies and approaches to cleanup that will solve the technically complex problems facing the government's largest environmental cleanup program. Additional information on the EMSP can be found at http://emsp.em.doe.gov.

Water Travels Chaotically through the Ground

Water flows in mysterious ways. Lawrence Berkeley National Laboratory hydrogeologist Boris Faybishenko has discovered that the mystery of water flowing through the earth can be explained using chaos theory. Using this theory, he and his colleagues may be better able to model how water – and therefore waterborne contaminants – seeps from the earth's surface to the water table below.

Current modeling methods can predict water movements through the ground fairly well, if limited to homogenous soils such as sand. Many sites with radioactive or organic contaminants, however, such as the Department of Energy's Hanford and Savannah River sites and the Idaho National Engineering and Environmental Laboratory, sit on heterogeneous soils or fractured rock. "Heterogeneous soils are the rule rather than the exception," said Faybishenko.

In these mixed soil or fractured rock environments between the earth's surface and the water table, said Faybishenko, water flow processes are non-linear and chaotic – that is, small differences in the system's initial conditions can lead to large differences later on in the system. Furthermore, different equations and models are needed to describe the water flow depending on the scale one chooses to examine. In a presentation to the Fall 1998 American Geophysical Union Meeting in San Francisco on December 10, Faybishenko proposed a hierarchic set of deterministic and stochastic, chaotic models to describe water flow through fractured rock.

Faybishenko and his colleagues, funded by the Department of Energy's Environmental Management Science Program, have investigated water movements at a range of scales. At the smallest scale, they studied water seeping between two glass plates. At the other end of the spectrum, a 1994 infiltration study led by Tom Wood title and a team of hydrologists from the INEEL tested water and short-lived radioactive tracer transport from a 6.5-acre pool through the underlying 600 feet of rock and soil to the aquifer below. Faybishenko and Wood first began to suspect that water flow through fractured rock might be a chaotic process when analyzing data from this large-scale test.

For about 15 years, Faybishenko had been keeping up with the scientific literature about chaos theory as a hobby. He expected to find applications of the theory in hydrogeology, and when he began working on field experiments in Idaho, his interest and knowledge reached a "critical mass," he said. Since then, he has returned to past data sets and found more evidence of chaotic behavior.

Faybishenko's collaborators at the INEEL have performed extensive field studies of water flow through fractures in basalt at small (less than one meter) and intermediate (ten meter) scales. "The 100-meter scale is much easier to understand and model because of averaging properties in fractured rock," said Tom Stoops of the INEEL. "But the 10-meter or smaller scale," he said, "is crucial for environmental restoration." Gasoline stations, waste burial pits, and many spills are governed by the small-scale properties that the group is learning to characterize using chaos theory. "Clean-up takes place at the meter scale, one barrel at a time," said Stoops.

In order to uncover the chaotic equations that describe water flow at this scale, 5,000 or more data points must be collected, said Rob Podgorney, a Senior Engineer at the INEEL. To generate all this data, the team spent last summer tracking water dripping through several fractures at Hell's Half Acre, a lava field outside of Idaho Falls. Because their approach combined the precision of a laboratory experiment with the real-world conditions of a field study, the INEEL researchers had to make or adapt many of the instruments they used for the tests. Water seeped from an artificial pond (whose level was maintained by a converted motorcycle carburetor) through a fracture in an overhang. Below, 20 sensors (using the same

pressure sensor technology that makes kids' tennis shoes light up with each step) recorded the time and location of drips leaving the fracture. The innards from a laboratory balance measured the outflow of water along different portions of the fractures.

Strangely, subsequent experimental trials gave different results although the starting conditions were seemingly identical. The researchers kept track of temperature, humidity, flow rate, soil water pressure, and other variables – but nothing they measured could account for the wide variation of final results. "All of my training and experience suggested that if you do the exact same thing, again and again, the results should be fairly consistent," said Wood. "But they weren't."

This pattern of apparent unpredictability is a hallmark of chaotic systems. However, once the right equations are found – a process that may require a lot of ingenuity and computer time – they can predict the range of possible outcomes given a set of starting conditions. Faybishenko has already uncovered equations that describe the pattern of fractures in basalt and the trajectory of flow paths in the basalt. These non-linear equations also describe chaotic systems that have been discovered in biology, chemistry, and atmospheric sciences. "It's all the same nature," said Faybishenko.

When Faybishenko and his colleagues find the best equations to describe water flow at the appropriate scales, their hierarchical model may help guide waste remediation efforts and environmental monitoring. With the best models in hand, environmental restoration stands the best chance of stopping contamination before it steals into the water table.

Laser Razor Shaves Radioactive Contamination from Skin of Buildings

Scientists at the Department of Energy's Argonne National Laboratory have designed a system to remove and collect radioactively contaminated concrete surfaces from a building without having to dismantle and dispose of the entire structure. The system uses a powerful laser to remove the thin layer of contaminated concrete, and another smaller laser to identify the chemical and radioactive composition of the material removed.

Throughout the country many radioactively contaminated buildings await the wrecker's ball—research facilities, sites where nuclear fuel rods were made, temporary nuclear storage structures, as well as aging nuclear power plants. The expense lies in the need to take thousands of samples for analysis – first to find out what is contaminated, and then after clean-up to ensure that all the contamination has been removed.

But in much of the concrete only the surface and a thin layer underneath are radioactive. Dismantling the entire building is like throwing away an apple because the skin is dirty. Scientists at the Argonne National Laboratory is searching for a more economical method of decontamination. "If you were lucky," said Michael Pellin, senior chemist and group leader for the project, "you could use the building, clean it up and return it to the lab for use again."

Pellin and his colleagues Keng Leong and Michael Savina tried to find where and how radioactive elements penetrate concrete, and whether a powerful laser could dislodge contaminated material. They first tested the laser ablation (removal) system on samples of concrete from a reactor at Argonne, and on concrete made in the laboratory and spiked with the element cesium. "The aim was to design an on-site removal and analytical method to determine that you have removed the contaminated material," said Pellin.

The laser beam—intense, amplified light—travels through a fiber optic cable and passes back and forth across the surface of the concrete. As the laser vaporizes the concrete, a vacuum-housing around the cable sucks up the removed material. Pellin describes the technology as a "fiber-optic light-pipe with a vacuum cleaner around it," and adds "it's a laser razor." After shaving off material, the researchers could analyze what they had gathered and what was left.

A laser beam only half a millimeter in diameter produces temperatures of more than 1500 degrees Celsius—melting some particles, vaporizing others, and disaggregating the concrete. Old concrete disintegrates faster (or more quickly) than new material, and exterior concrete disintegrates easier than the stuff inside the samples. In the process Pellin and his team discovered that contamination was not as deep in the pebbles and gravel of the concrete as it was in the matrix that held those grains together.

Savina explains that they need to know how radioactive contamination penetrates into walls and floors and how it diffuses in the matrix of the cesium-spiked concrete they made. "Understanding the chemistry of radioactive ion mobility (into concrete) is important in designing future buildings that will make this work unnecessary," said Pellin. Secondary ion or sputtered ion mass spectrometry helps him and his colleagues gain that understanding. One laser vaporizes the surface of the sample, and another—aimed above the surface so as to hit the escaping material—converts atoms to charged particles or ions. Passed through an electrical field, the different ions travel at different velocities and can therefore be identified in a time-of-flight mass spectrometer.

With a detection limit lower than one part per million, the mass spectrometer showed that a single pass with the laser razor can produce a thirty to three hundred-fold reduction in the amount of cesium in spiked

samples, more than enough to reduce contamination to below levels defined as safe. "Before we design an instrument for the field, we need to know how sensitive we need to be," Savina said, "and we need to analyze the effluent to know what to remove." Knowing what to remove is the key to lowering the cost of cleanup.

"We have to go to just the right depth in the wall," said Pellin. "This reduces costs in two ways. We can prove it is clean, and we reduce the volume of material you have to get rid of." Going to the right depth is especially difficult in some older buildings where the walls are covered with lead paint. "Material that is chemically toxic and radioactive at the same time," said Pellin, "is recognized as very difficult to dispose of. What we would do is use the laser razor to remove the paint first."

Although the laser razor is more expensive to use than a paint scraper, Savina explained that if the razor and the analytical system are combined and used together, "there will be a tremendous savings in time and dollars. We hope to bring this instrument on line, then to have a company come in and develop it commercially."

This research is designed to uncover where the impurities in contaminated material are and where the radiation has gone. "Just to know *that* is grist for the mill for doing this better. I am excited about working on a project that studies a huge problem that needs to be fixed," said Pellin. Savina is equally enthusiastic. "We are contributing to cleaning up a horrendous environmental mess," he said, "and what captures me is the nature of the project, from industrial scale to very sophisticated science. We have a monster laser that can disaggregate concrete. We have another laser that can pick apart the material into tiny micron size particles and analyze every different atom that is in the material."

This work is supported by the U.S. Department of Energy Environmental Management Science Program (EMSP). The EMSP funds basic research through a partnership between the Office of Environmental Management (EM) and the Office of Science (SC) in the Department of Energy. The intent of the EMSP is to develop the scientific knowledge needed to create new technologies and approaches to cleanup that will solve the technically complex problems facing the government's largest environmental cleanup program. Additional information on the EMSP can be found at http://emsp.em.doe.gov.

Improved Neutron Technology for Identification of Nuclear Waste

Scientists at Los Alamos National Laboratory are developing an analytical tool that will increase by a thousandfold their ability to analyze and measure contaminated and heterogeneous nuclear materials being prepared for permanent disposal.

This work is supported by the U.S. Department of Energy Environmental Management Science Program (EMSP). The intent of the EMSP is to develop the scientific knowledge needed to create new technologies and approaches to cleanup that will solve the technically complex problems facing the government's largest environmental cleanup program.

Improved analytical technology is essential to ensure the safe storage of nuclear materials, which include radioactive elements, and non-radioactive toxic elements such as mercury, cadmium and lead. The Resource Conservation and Recovery Act (RCRA) of 1976 defines what hazardous materials must be isolated and how to dispose of them. In order to comply with the RCRA, scientists must identify and classify the materials produced during nuclear operations.

Fortunately, all the radioactive and toxic elements in typical mixed nuclear waste can be analyzed by one method: bombardment by neutrons, nuclear particles with no charge. Under such bombardment, the nuclei of atoms of the radioactive elements are fissile—they split—and give off more neutrons, which can be detected to identify the radioactive material. The toxic, non-radioactive elements give off characteristic gamma rays when hit by neutrons, and can also be identified.

"The more neutrons you can bombard with, the easier you can see smaller and smaller quantities," said Mark Pickrell, deputy group leader of the Safeguard Science and Technology Group at Los Alamos. The "High-Fluence Neutron Source", the new design from Los Alamos, will increase the flow from one hundred million to one hundred billion neutrons per second, a thousandfold improvement. "Now," added Pickrell, "one milligram of plutonium can be measured in a 55 gal. drum." That's less than one part per million.

The improved analytical capability is necessary because the standards for disposal of dangerous materials are becoming more and more stringent. Furthermore, some radioactive waste is stored temporarily in sealed drums that contain water. Water's hydrogen acts as a shield to neutrons, and to break through that shield, the flow of neutrons has to be increased.

Neutron technology can identify alpha radiation, which from the biological point of view is the most hazardous radiation of all. Alpha radiation is a stream of alpha particles, which are the nuclei of atoms of helium. "Think of the alpha particle," said Pickrell, describing the danger of inhalation of these particles, "as the bowling ball of nuclear physics. It is big and charged. It stops as soon as it hits matter, and deposits its energy." That energy damages and ultimately destroys living tissue.

"But," said Pickrell, "by a peculiar piece of serendipity, all the nuclear materials that emit alpha particles are fissile. So one method of measuring alpha-emitters is to bombard them with neutrons and detect the fissions."

The High-Fluence Neutron Source creates a great flow of neutrons from high-speed collisions of deuterium and tritium, the less-common forms of the element hydrogen. Earlier designs created these collisions, but not at a sufficient velocity to generate enough neutrons. The new Los Alamos design creates tightly focussed beams of deuterium and tritium that collide at high velocity at the center of an evacuated spherical chamber to generate the greatest number of neutrons.

Pickrell sees the technology being used in several sites around the country. Drums of nuclear waste would be shipped in for assay and then disposed of according to their classification after the analysis is complete.

The new neutron technology could also be used in mining, where there is a need for constantly monitoring the quality of the product or ore. As coal, for example, or mined ore passed by on a moving belt, the material could be analyzed in a beam of neutrons, allowing instantaneous quality control. Operators could determine the ash or sulfur content of coal and then after analysis blend mixes of coals to produce the most desirable combination for energy content and environmental suitability.

The High-Fluence Neutron Source has attracted some commercial interest. "What we would like," says Mike Hurwitz, a scientist at GAMMA-METRICS, a San Diego company that specializes in using neutrons for analysis, "is a neutron source that we can turn on and off, and that has a long life, that is, more than 10,000 hours." The new design from Los Alamos meets those requirements, and Hurwitz believes that the work at Los Alamos "has the potential for a technological breakthrough that may lead to a simple, commercial version."

The U. S. Department of Energy Environmental Management Science Program funds basic research through a partnership between the Office of Environmental Management (EM) and the Office of Science (SC) in the Department of Energy. Additional information on the EMSP can be found at http://emsp.em.doe.gov.

Engineering Plants for Bioremediation of Mercury

For the most part, plants just sit there in the sunshine—sucking in nutrients from the soil, transmitting the nutrients through their plant tissues to be metabolized, and dispatching the byproducts into the air through their leaves. But aided by a couple of genes from bacteria, the placid plants may eventually clean up toxic metals in soils, marshes and rivers.

Researchers at the University of Georgia have engineered an assortment of flowering plants, including yellow poplar and tobacco, to extract toxic mercury compounds from contaminated soils, convert them into less toxic forms and either expire the end product into the air or sequester it in their leaves. "What we are doing is what plants are designed to do—extract chemicals from soil," said plant geneticist Richard Meagher. "And, fortunately, the sun provides the raw energy to do that."

Pervasive across the United States and in many other parts of the world, mercury contamination of soil and water persists due to ineffective clean-up methods. Both industrial and government activities have contributed to the contamination. For example, mercury has been used in bleaching processes, in some agricultural pesticides, and as a coolant in nuclear power plants.

Mercury appears in the environment as metallic or ionic. These two forms present little hazard of moving in the food chain and poisoning animals—only a small percent of the mercury is absorbed by organisms in each step of the chain.

However, ionic mercury can be easily converted by many bacterial species into methylmercury, a toxin that causes dementia in low doses—the "Mad Hatter" is said to have suffered from mercury-induced lunacy because of the chemical's use in felting processes. Low doses of methylmercury are concentrated into much higher doses as the toxin moves up the food chain. Fish and carnivorous animals can have a million to a hundred-million times more methylmercury in them than originally found in the soil.

Meagher has been using experimental plants to remove mercury from mercury-spiked laboratory plant food and mercury-spiked soil. His group has successfully engineered tobacco, yellow poplar, and arabidopsis, a small plant related to cabbage that is easily manipulated by genetics researchers, to convert methylmercury into the less toxic ionic mercury, and to convert the ionic mercury into metallic mercury, a relatively non-toxic element that is released by the plants into the environment. His poplar results appeared in the journal Nature Biotechnology in October, 1998.

Meagher wants to customize plants for different environments. His group is now trying to engineer rice and spartina, a common marsh grass, to remediate mercury from marshy, wet areas. Funded by the Department of Energy's Environmental Management Science Program, the project will produce engineered plants that will be useful for many of the DOE's contaminated sites.

Normally, plants growing in mercury-contaminated soils accumulate ionic and methylmercury in their roots. The plants are sensitive to the concentration of mercury and often can't grow if it is above 50 parts per million.

Two genes from bacteria, though, enable the plants to modify the forms of available mercury. The Georgia researchers have successfully transferred these genes to various plants and tested how well the plants resist high concentrations of toxic mercury and convert it.

One gene, merB, converts methylmercury into ionic mercury. The second, merA, converts ionic mercury into metallic mercury, which is volatile and escapes from the plants as gas. Metallic mercury is the safest form of mercury—on its own, it is relatively non-reactive with other chemicals, isn't easily converted into methylmercury and doesn't get concentrated as it moves up the food chain. Also, said Meagher, blowing metallic mercury off as gas is the EPA-approved method of mercury clean-up.

It is possible to turn off merA in the leaves but leave it on in the roots. Meager said that the leaves would accumulate high levels of ionic mercury and could be harvested for the metal. However, harvesting the mercury in this way is not yet profitable, he said.

Plants that manage mercury using the bacterial genes provide valuable advantages over current methods of remediation. Heavily contaminated sites, Meagher said, have concentrations of mercury of 100 to 1000 parts per million. The engineered plants could convert mercury at these concentrations to metallic gas and require minimal management while doing it.

Even more important for mercury remediation, though, is the root system of plants. "The roots can provide a surface area of 100 million miles per acre of soil," said Meagher. "No engineered remediation scheme could ever afford to generate that much surface area available for extraction."

Plus, said Meagher, "Plants are aesthetically pleasing."

Meagher hopes to develop the bio-engineered plants at a tenth of the cost of current remediation methods. "For this method to catch on, it has to be cheaper," he said. "I don't think people will pay for it unless it pays for itself."

The costs include transferring the two genes into the plants and then growing the seeds that contain the bacterial DNA and testing them. In addition, genes in plants work slightly differently than genes in bacteria. Like putting a Ford truck's carburetor into a Nissan sedan, modifications have to be made to the genes for them to work properly.

So far, the flowering plants that Meagher's group has engineered have worked well. Rice and spartina, however, are proving more difficult. Rice and spartina are different kinds of flowering plants, called monocots, than the tobacco and poplar, which are dicots. Monocots are more difficult to genetically engineer—they grow and reproduce slower in the laboratory.

The monocots, Meagher said, will take six months to engineer and three more months to harvest seeds from. "We have to dissect 1000 seeds to get five that give embryos," he said. "They are not the ideal plants for genetic engineering, but they are the ideal plants for bioremediation."

Fact Sheets

FACT SHEETS

This section includes project summaries from selected EMSP projects. These projects were selected as part of a special evaluation that was implemented to identify projects that were promising from a commercialization perspective. This evaluation was focused primarily on the projects in the EMSP portfolio that were in more mature stages of development and therefore did not consider many of the newer projects that were started after 1996.

FACTS ON FILE

Development of Inorganic Ion Exchangers for Nuclear Waste Remediation

Problem Area: High Level Waste

Scientific Category/Subcategory: Separations Chemistry/Ligand Design and Ion Exchange

Description: Researchers at Texas A&M University and Oak Ridge National Laboratory are exploring highly selective inorganic ion exchanger materials for removal of primarily cesium and strontium from nuclear tank waste and from ground water. They are undertaking detailed structural studies on a variety of materials including cavity, layered and amorphous gel structures to elucidate the thermodynamic, kinetic, and molecular basis for ion exchange.

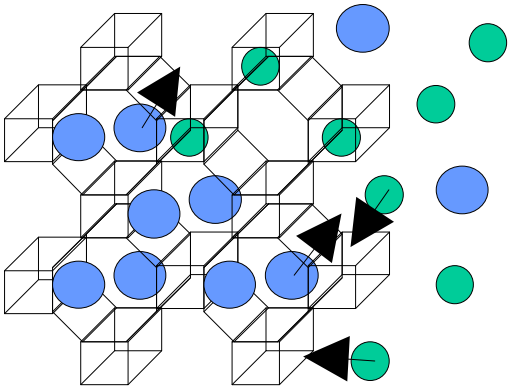
Application: These studies are most applicable to the Tanks Focus Area, but also potentially to the Mixed Waste and Subsurface Contaminants Focus Areas, since it can lead to improved selectivity ion exchange materials for a host of contaminants. Improved ion exchangers can directly benefit separations efforts on high level waste at Richland, Savannah River, and Idaho to separate out the most radioactive constituents for vitrification.

Value/Benefits: Through better understanding the mechanisms and drivers of ion exchange processes, better ion exchange materials can be custom designed and engineered to function in complex ionic media for which current ion exchangers are not efficient or cost effective. Improved ion exchange selectivity can reduce the cost and complexity of separations processes, and thereby reduce the inherent risk to workers.

Project Lead:
Texas A&M University
Dr. Abraham Clearfield
(409) 845-2936 pjf2434@acxrd.chem.tamu.edu

Other Participating Institutions:
Oak Ridge National Laboratory
Dr. Zane Egan (423) 576-6068

Project Duration: 1996-1999



Web Information Sources:

http://emsp.em.doe.gov/portfolio/multisearch.asp

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FACTS ON FILE

Determining Significant Endpoints for Ecological Risk Analysis

Problem Area: Health/Ecology/Risk

Scientific Category/Subcategory: Health Science/Risk Assessment

Description: Researchers at Savannah River Ecology Center, the University of Puerto Rico, and Colorado State University are exploring protocols for assessing risk to non-human populations exposed to environmental stresses typically found on many DOE sites. For ecological risk assessments, the proper endpoint is much debated because the appropriate unit of interest for non-humans may not be individuals; risk might be assessed more properly at higher levels of biological organization, such as the population, community, or ecosystem.

Application: The information and techniques developed from this project will be applicable to all DOE sites where contaminants have been released to the environment and potentially may impact the indigenous flora and fauna. In particular the results will be applicable to the Savannah River Sites where current field experiments are taking place on model organisms.

Value/Benefits: The project represents cutting-edge research in risk analysis of ecological systems. Until recently, techniques development and application for ecological risk analysis would have required a monumental effort for each organism studied. It is now possible to achieve the same goal with much less effort in isolating the necessary probes by searching for chromosomal aberrations and determining metabolic rates in the selected organisms.

Project Lead:
Savannah River Ecology Laboratory
Dr. Thomas G. Hinton
(803) 557-7454 tom.hinton@srs.gov

Other Participating Institutions:
Colorado State University
Dr. Joel Bedford (970) 491-7492
University of Puerto Rico
Chris Rowe (787) 764-0000

Project Duration: 1996-1999

Web Information Sources:

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Containment of Toxic Metals and Radionuclides in Porous and Fractured Media: Optimizing Biogeochemical Reduction versus Geochemical Oxidation

Problem Area: Remedial Action

Scientific Category/Subcategory: Biogeochemistry/Biogeochemistry

Description: Researchers at Oak Ridge and Pacific Northwest National Laboratories and Florida International Univ. and Univ. of Idaho are exploring ways to render dissolved metal contaminants less mobile and less toxic by altering their redox state through natural biological underground processes. Metal ion oxidation state has a direct relationship to solubility and toxicity for metals such as uranium, chromium and cobalt, and therefore impacts their fate and transport in the environment.

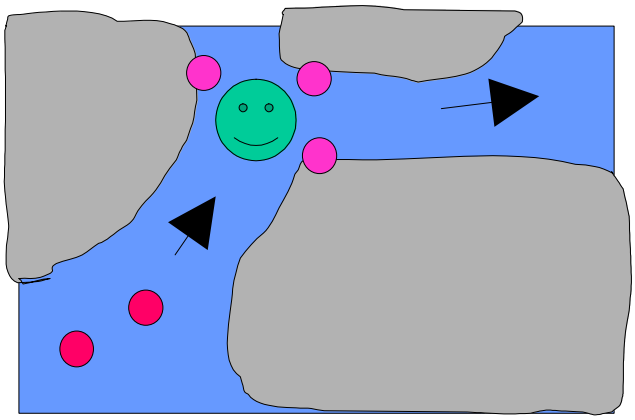
Application: The information and techniques developed from this project will be applicable to the Subsurface Contaminants Focus Area, and will ultimately lead to better understanding and enhancement/ optimization of these natural biological mechanisms. Potential sites where this may be applied include Savannah River's Old Burial Grounds, and Oak Ridge's Y-12 site where Cr, Co and U metals are present in the groundwater.

Value/Benefits: Through improved understanding of these biological mechanisms improved bioremediation techniques can be developed to cost effectively address metal contaminants in situ versus the more costly and long timeframe baseline technique of pump and treat.

Project Lead:
Oak Ridge National Laboratory
Dr. Philip M. Jardine
(423) 574-8058 ipj@ornl.gov

Project Duration: 1996-1999

Other Participating Institutions:
Florida International University
James Saiers saiers@fiu.edu
Stanford University
Scott Fendorf



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Design and Synthesis of the Next Generation of Crown Ethers for Waste Separations: An Inter-Laboratory Comprehensive Proposal

Problem Area: High-Level Waste

Scientific Category/Subcategory: Separations Chemistry/ Ligand Design and Ion Exchange

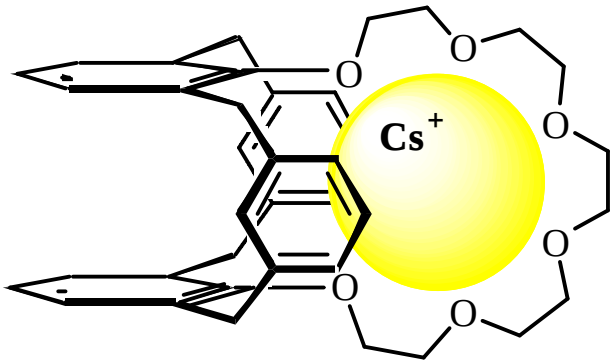
Description: Researchers at Oak Ridge, Argonne, and Pacific Northwest National Laboratories and University of Tennessee are combining molecular modeling and sophisticated synthesis techniques to provide a new generation of crown ethers for metal ion separation. This consists of three inter-dependent projects dealing with 1) molecular mechanics modeling and ligand design, 2) solvent-extraction properties, and 3) resin-immobilized crowns. Crown ethers and this research offer highly selective separations under difficult chemical environments.

Application: The information and techniques developed from this project will be applicable to the Tanks and Subsurface Contaminants Focus Area. Target problems include Li ions leaching from burial sites at Oak Ridge, and effective separation of Sr and Cs from contaminated high level waste at various DOE tank storage sites.

Value/Benefits: Improved synthesis techniques have been developed for new calix[4]arene crown ethers for potential Cs removal from high level wastes, resulting in potentially improved separation performance and ultimately lower separation costs. The project has significant near-term deployment potential and potential applications outside of EM.

Project Lead:
Oak Ridge National Laboratory
Dr. Bruce A. Moyer
(423) 574-6718 moyerba@ornl.gov

Other Participating Institutions:
Argonne National Laboratory
Mark L. Dietz mark_dietz@gmgate.anl.gov
Pacific Northwest National Laboratory
Benjamin P. Hay ben.hay@pnl.gov
University of Tennessee
S. Alexandratos alexsd@utk.edu



Project Duration: 1996-1999

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FACTS ON FILE

High-Fluence Neutron Source for Nondestructive Characterization of Nuclear Waste

Problem Area: Mixed Waste

Scientific Category/Subcategory: Analytical Chemistry and Instrumentation/Sensors and Techniques

Description: Researchers at Los Alamos National Laboratory are developing a high intensity neutron source (about 1,000 times more powerful than current capabilities) for nondestructive assay of containerized transuranic (TRU) waste. This new design for a neutron source is based on the inertial electrostatically confined (IEC) plasma device. Although the concept using a single grid for confinement has been around for nearly 3 decades, it has suffered from high plasma density, marginal neutron output, and limited lifetime due to neutral particle sputtering. The new IEC design has already resulted in lower plasma density, which should provide a significant increase in measurement sensitivity at a similar cost, weight and size to today's commercially available systems.

Application: These studies are applicable to the Mixed Wastes Focus Area, and to characterization of wastes targeted for WIPP such as remote handled, cemented or vitrified wastes, spent nuclear fuel, and other streams resulting from processing of high level waste. In particular, this technology could benefit a variety of sites/facilities including the Advanced Mixed Waste Treatment Project, Consolidated Incinerator Facility, and Idaho Chemical Processing Plant.

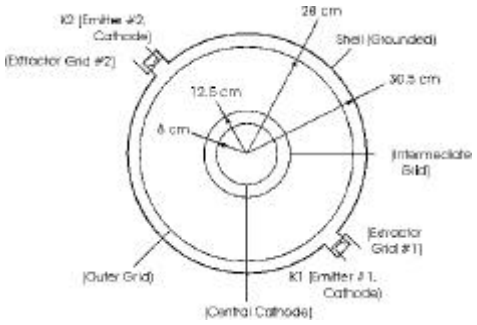
Value/Benefits: The essential features of the IEC plasma source are high neutron flux, long lifetime, and the option for pulsed or steady-state operation modes. This provides increased characterization sensitivity and flexibility, thereby increasing production rates and cost savings. Cost savings also result from the ability to better distinguish low level from TRU wastes and the associated disposal costs associated with each type of waste.

Project Lead:
Los Alamos National Laboratory
Dr. Mark Pickrell
(505) 665-5098 mpickrell@lanl.gov

Project Duration: 1996-1999

Web Information Sources:

http://emsp.em.doe.gov/portfolio/multisearch.asp



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Seismic-Reflection and Ground Penetrating Radar for Environmental Site Characterization

Problem Area: Remedial Action

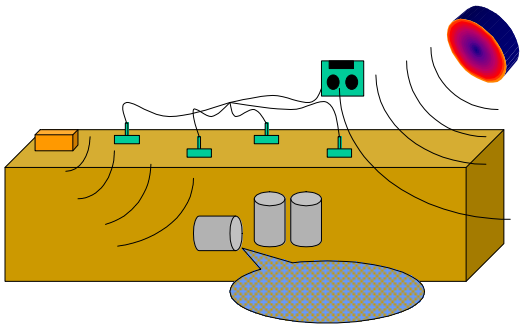
Scientific Category/Subcategory: Geophysics/Subsurface Imaging

Description: Researchers at the University of Kansas are marrying two well developed technologies for non-intrusively characterizing shallow subsurface features (2 to 8 meters) of suspected waste sites. The first is seismic reflection employing high dynamic range and multi-channel vibratory signals with close spaced geophones to map the near surface. The second technique employs ground penetrating radar (high frequency radio waves) that can probe shallow distances in to the soil. The reflections from each type of wave provides unique information that when combined and computer enhanced allow much greater detail as to the size and extent of buried wastes and associated plumes.

Application: The information and techniques developed from this project will directly improve the capabilities of the Subsurface Contaminants Focus Area for characterizing waste burial sites and devising cost effective strategies to address the cleanup. In particular this technology should address characterization needs associated with remedial actions in the 100, 200 and 300 Areas at Richland, and at the Idaho Chemical Processing Plant which are high risk, planned actions to be addressed in the 2007 and beyond timeframe.

Value/Benefits: Current baseline characterization technology for suspected burial sites involves invasive processes such as drilling which is time consuming, costly, provides only a limited view of the larger picture, and has the potential to exacerbate the problem. Therefore successful development of this combined characterization and computer enhancement technique provides not only time and cost savings, but also improved synergistic knowledge for devising an effective remediation strategy with minimal further threat to the environment or workers.

Project Lead:
University of Kansas
Dr. Don W. Steeples
(785) 864-2730 steeples@kuhub.cc.ukans.edu



Project Duration: 1997-2000

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